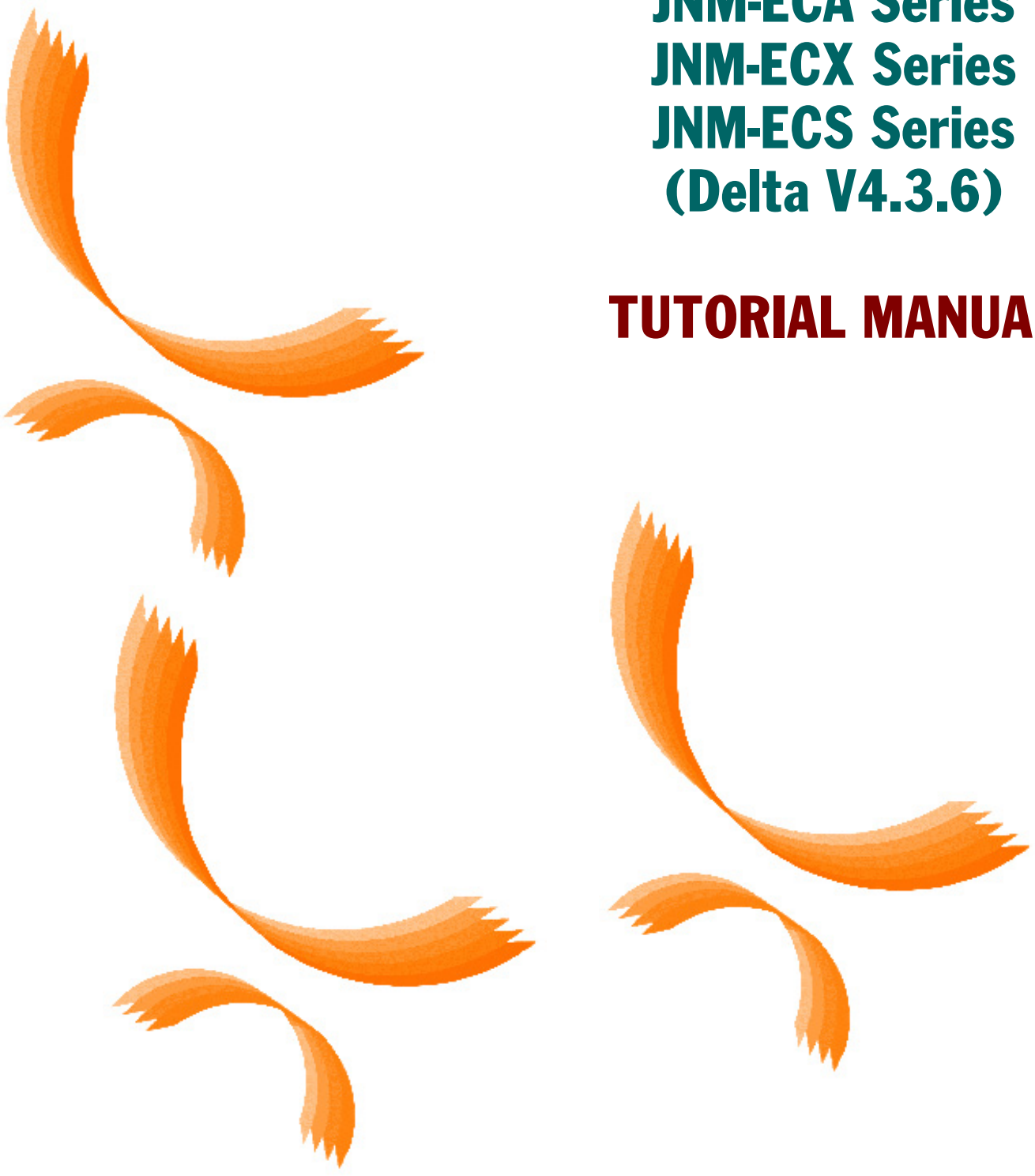
JNM-ECA Series
JNM-ECX Series
JNM-ECS Series
(Delta V4.3.6)

TUTORIAL MANUAL



INMECA/ECX-TU-3a
AUG2007-08110235
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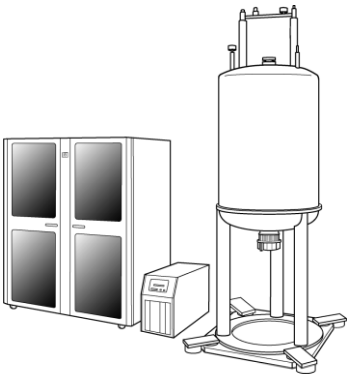
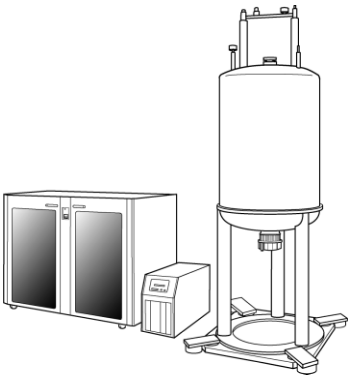
JNM-ECA Series
JNM-ECX Series
JNM-ECS Series
(Delta V4.3.6)

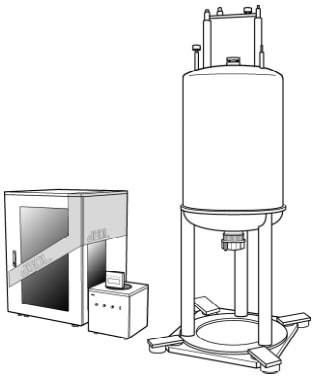
TUTORIAL MANUAL



JNM-ECA Series



JNM-ECX Series



JNM-ECS Series

This manual is designed for new users of the JNM-ECA, JNM-ECX or JNM-ECS Series FT NMR system who want to perform 1D or 2D NMR measurement. It explains the basic procedures for operating the system. For details of individual operations, refer to the on-line “User's Manual".

Please be sure to read this instruction manual carefully, and fully understand its contents prior to the operation or maintenance for the proper use of the instrument.

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NOTATIONAL CONVENTIONS AND GLOSSARY

General notations

– CAUTION – :	Points where great care and attention is required when operating the device to avoid damage to the device itself.
✍ :	Additional points to be remembered regarding the operation.
☞ :	A reference to another section, chapter or manual.
1, 2, 3 :	Numbers indicate a series of operations that achieve a task.
◆ :	A diamond indicates a single operation that achieve a task.
File:	The names of menus, commands, or parameters displayed on the screen are denoted with **bold** letters.
File–Exit :	A command to be executed from a pulldown menu is denoted by linking the menu name and the command name with a dash (–). For example, **File–Exit** means to execute the **Exit** command by selecting it from the **File** menu.
Ctrl :	Keys on the keyboard are denoted by enclosing their names in a box.

Mouse operation

Mouse pointer:	An arrow-shaped mark displayed on the screen, which moves with the movement of the mouse. It is used to specify a menu item, command, parameter value, and other items. Its shape changes according to the situation.
Click:	To press and release the left mouse button.
Double-click:	To press and release the left mouse button twice quickly.
Drag:	To hold down the left mouse button while moving the mouse. To drag an item, you point to an item on the screen and then drag it using the mouse.

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1

PREPARATION FOR MEASUREMENT

Chapter 1 explains the startup and shutdown of the Delta program, sample setup, sample loading, NMR lock, automatic resolution adjustment, and other operations to be carried out prior to measurement.

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1.1 STARTING AND EXITING THE DELTA PROGRAM

This section assumes that the data system has started normally, and that the login operation is complete.

☞ For starting the data system and login, refer to the separate manual on the workstation.

■ Starting the Delta program

◆ Double-click on the **Delta** icon on the screen.

The Delta program starts, and the **Delta Console** window opens.

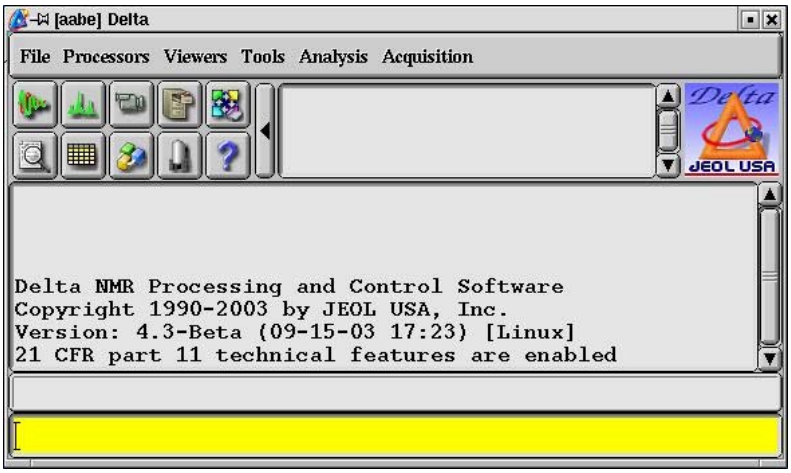
[aabe] Delta
File Processors Viewers Tools Analysis Acquisition
Delta
JEOL USA
Delta NMR Processing and Control Software
Copyright 1990-2003 by JEOL USA, Inc.
Version: 4.3-Beta (09-15-03 17:23) [Linux]
21 CFR part 11 technical features are enabled

Fig. 1.1 Delta Console window

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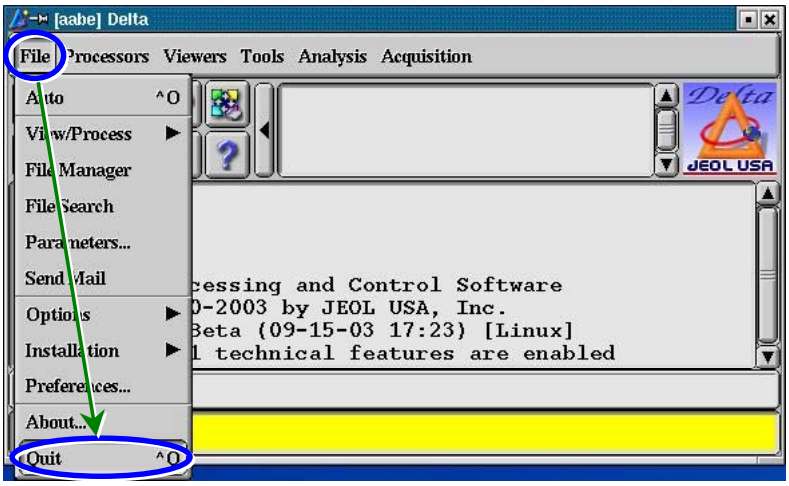
Ending the Delta program

After measurement or NMR data processing is complete, terminate the Delta program as follows.

1. Select **File–Quit** in the **Delta Console** window.

First, point to **File** in the menu bar in the **Delta Console** window, and press and hold the left mouse button. A pull-down menu appears. Then, while holding down the left mouse button, move the mouse to highlight **Quit** in the pull-down menu, and release the left mouse button there**.**



Verify Quit. The **Confirm** window opens.

Fig. 1.2 Confirm window

2. Click on the **OK** button.

The Delta program ends.

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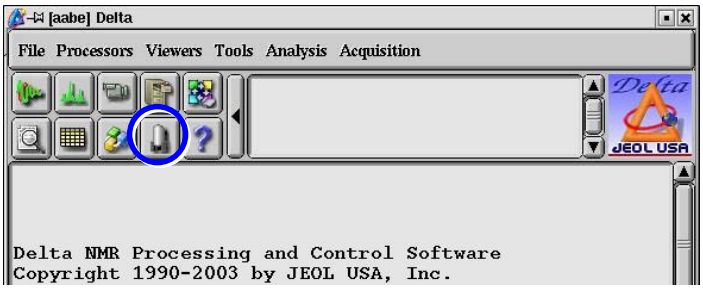
1.2 CONNECTING TO AND DISCONNECTING FROM A SPECTROMETER

The Delta program can be connected with two or more spectrometers through the network in the JNM-ECA/ECX series FT NMR instrument. For this reason, before NMR measurement, it is required to connect the Delta program with the spectrometer you will use. After NMR measurement, disconnect the NMR spectrometer from the Delta program. Here, we will explain how to connect and disconnect the Delta program and the NMR spectrometer.

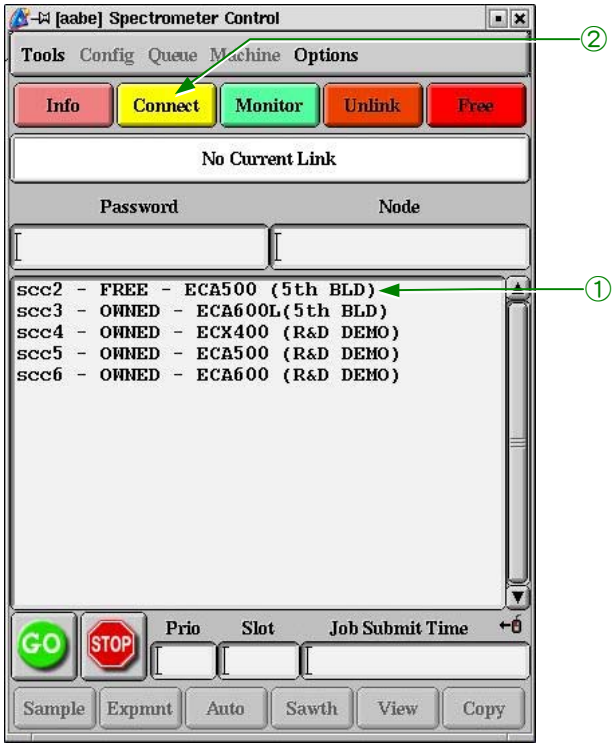
■ Connecting to the spectrometer

1. Click on the button in the **Delta Console** window.


[aabe] Delta
File Processors Viewers Tools Analysis Acquisition
JEOL USA
Delta NMR Processing and Control Software
Copyright 1990-2003 by JEOL USA, Inc.

The **Spectrometer Control** window opens, and a list of the currently available spectrometers appear in the list box (☞ Fig. 1.3).

The spectrometers which are marked as **FREE** are available for connection. The spectrometers which are marked as **OWNED** are currently being used.



✍ The numbers ① and ② are referred to in the following steps.

Fig. 1.3 Spectrometer Control window

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2. Using the mouse, select the spectrometer you want to connect to by clicking on its name in the list in the **Spectrometer Control** window (☞ ① in Fig. 1.3).

3. Click on the **Connect** button (☞② in Fig. 1.3).

If the connection is carried out correctly, the message "**Connect:** ⋯" is displayed in the **Spectrometer Control** window, as shown in Fig. 1.4.

Fig. 1.4 Spectrometer Control window after the spectrometer is connected

■ Disconnecting from the spectrometer

◆ Click on the **Unlink** button in the **Spectrometer Control** window.

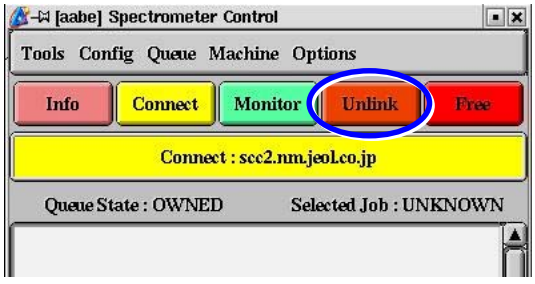

Fig. 1.5 Spectrometer Control window: Spectrometer is connected

When the spectrometer is disconnected, the **Spectrometer Control** window returns to the display shown in Fig. 1.3.

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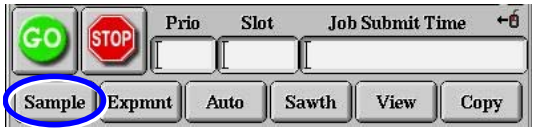
1.3 SAMPLE PREPARATION

This section explains how to insert the sample into the SCM.

1.3.1 Check Prior to Sample Insertion

Check to make sure that no other sample is inserted in the SCM as follows.

1. Connect to the spectrometer according to the procedure of Section 1.2.
2. Click on the **Sample** button in the **Spectrometer Control** window.



The **Sample** window opens.

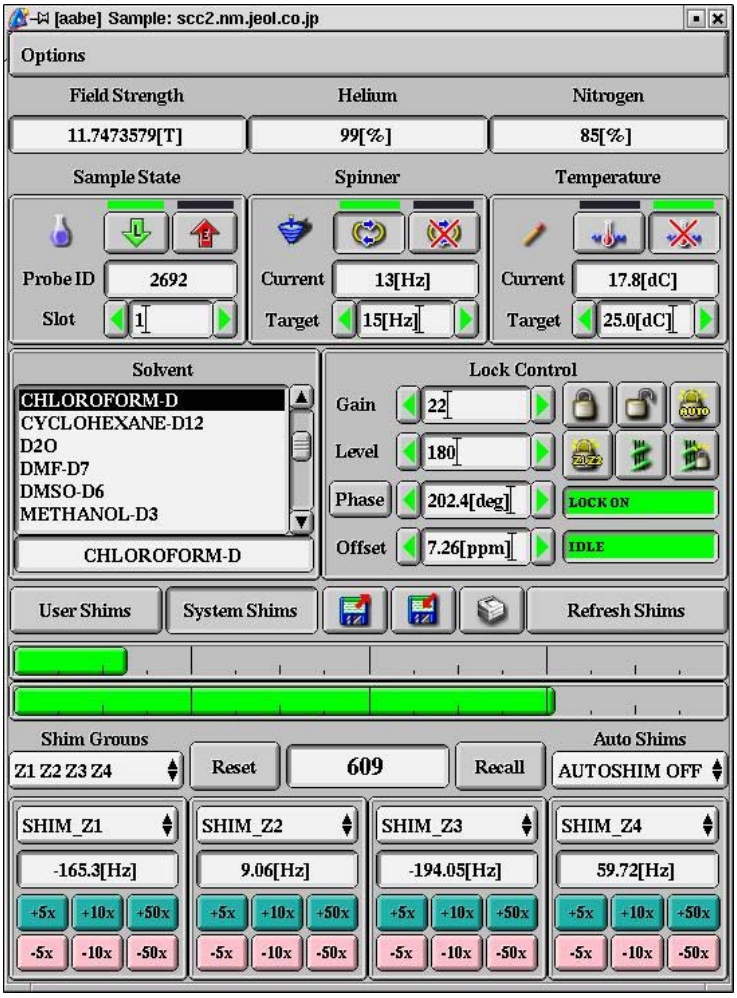


Fig. 1.6 Sample window

3. Verify that the **Sample State** section in the **Sample** window indicates that no sample is loaded.

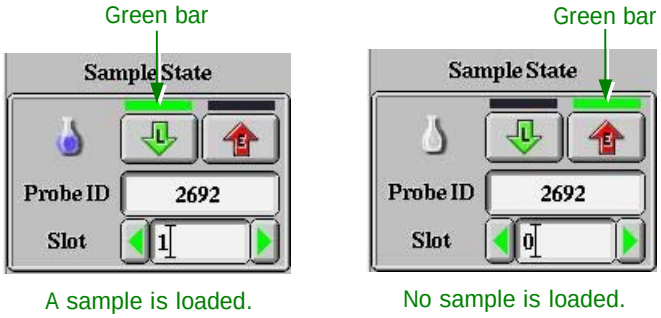


Fig. 1.7 Sample State

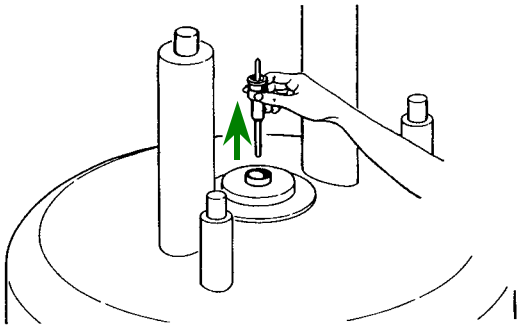
If the display shows that no sample is loaded, proceed to ■ Setting up the sample. If the display shows that a sample is loaded, remove the sample according to the procedure ■ Ejecting the sample.

■ Ejecting the sample

● When an auto sample changer is not installed.

If a sample is inserted in the SCM, remove it.

1. Click on the **Sample** button in the **Spectrometer Control** window to open the **Sample** window.
2. Click on the button.
   The sample in the SCM is ejected. Verify that the **Sample State** section indicates that the sample has been ejected.
3. Remove the sample from the insertion port on the SCM.



● When an auto sample changer is installed.

Another sample has been inserted into SCM, take out the sample according to the following procedure :

1. Open the **Sample** window.
2. Set the **Slot** number to 0.
   The sample can be ejected from the SCM, and is moved to the neutral position of the auto sample changer. At the same time, verify that the **Sample State** indicator changes to the ejected state.
3. Take the sample out of the slot of the auto sample changer.

■ Setting up the sample

⚠ WARNING

Be sure to wear protective gloves when handling a sample tube containing a poisonous sample. If the sample tube breaks, this allows you to avoid contact with any sample that leaks.

1. Set the sample tube (with the sample in it) in the holder.

Since the resolution varies according to the sample volume (height), it is recommended that you standardize the sample volume. An appropriate sample height is approximately 4 cm (3.8 to 4.2 cm).

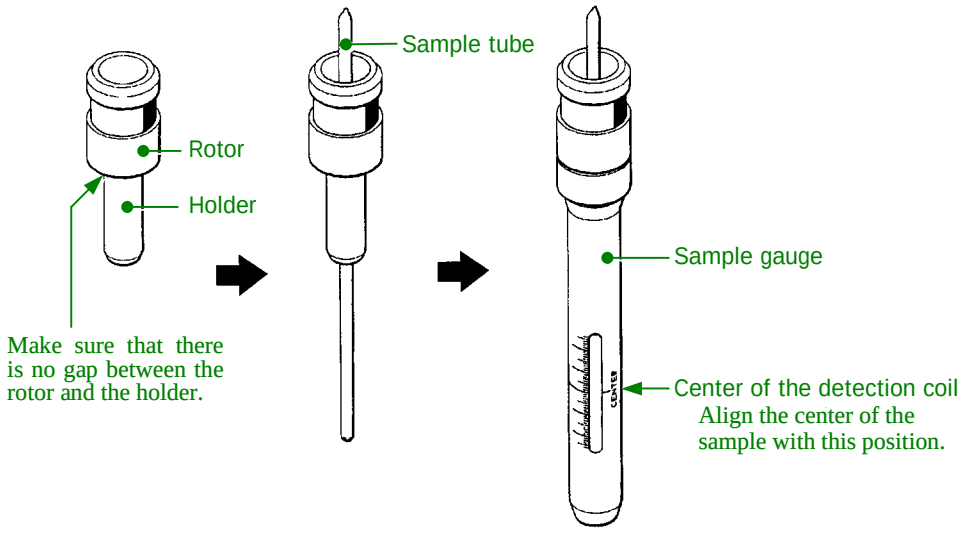

Sample tube
Rotor
Holder
Sample gauge
Make sure that there is no gap between the rotor and the holder.
Center of the detection coil
Align the center of the sample with this position.

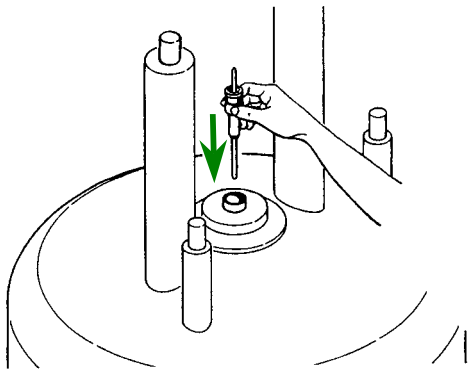
Fig. 1.8 Setting up the holder

2. Check to make sure that the air is flowing by holding your hand over the sample-insertion port of the SCM.

If air is not flowing, never insert the sample tube into the insertion port of the SCM. Another sample may already have been inserted or there might be a problem with the air system.

3. Put the sample, in the holder, into the sample-insertion port of the SCM and gently release it.

The sample levitates on the compressed air.



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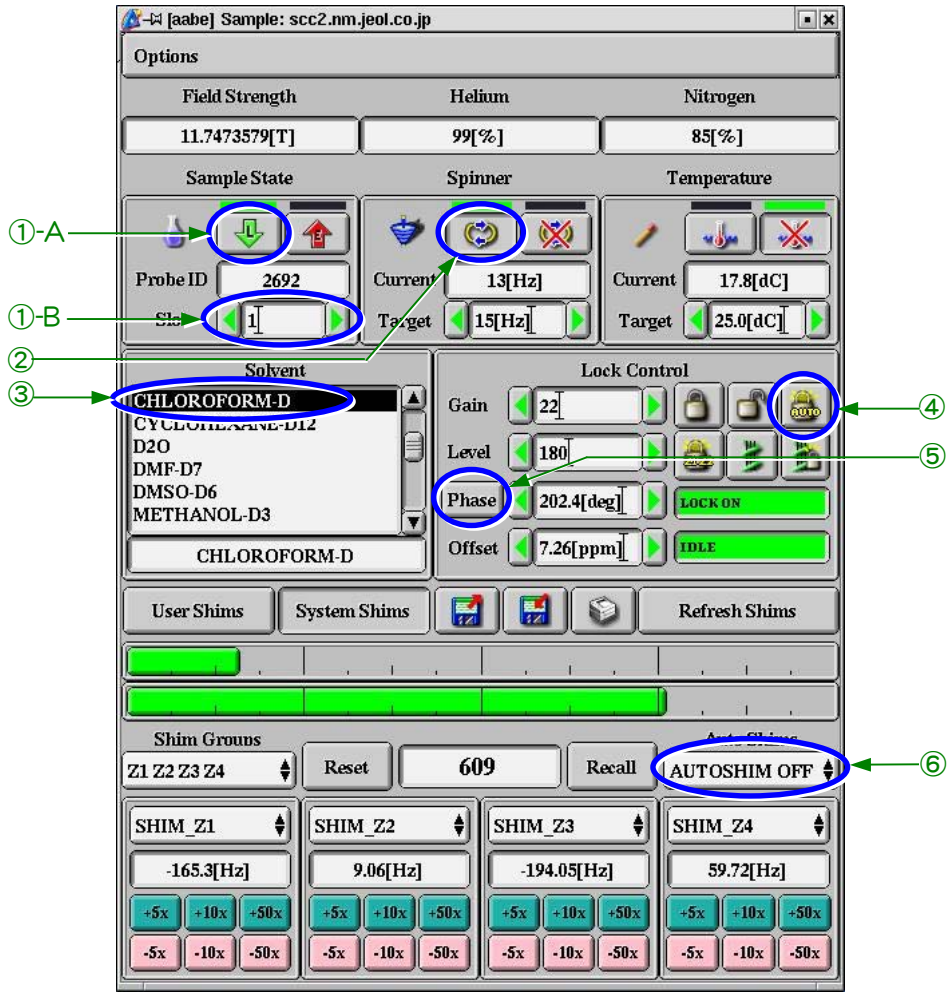
1.3.2 Sample Loading, NMR Lock, and Automatic Resolution Adjustment

Sample loading, NMR lock, and automatic resolution adjustment are performed using the **Sample** window.



✍ The numbers ① to ⑥ are referred to in the following steps.

Fig. 1.9 Sample window

■ Loading the sample

● When an auto sample changer is not installed.

Insert into the SCM the sample which was set in the sample-insertion port of the SCM.

◆ Click on the button in the **Sample** window (☞①-A in Fig.1.9).
When the sample load completes, the flask icon becomes full, as shown below.

● When an auto sample changer is installed

1. Set a sample to the slot of the auto sample changer.

2. Set the slot numbers place a sample of the auto sample changer into the **Slot** of the **Sample** window (☞①-B in Fig.1.9).

After carrying a sample to the top of the SCM, insert it into the SCM. When sample loading is complete, the flask display changes as follows :

■ Spinning the sample

Usually, you measure the sample while spinning it. If you want to measure the sample without spinning, proceed to ■**NMR lock**.

◆ Click on the button(☞② in Fig.1.9).

When the sample starts spinning, the toppled top will be upright as shown below.

■ NMR lock

Select the solvent to be used for NMR locking and execute the NMR lock command.

1. Select the solvent to be used for NMR locking from the **Solvent** list box (☞③ in Fig.1.9).

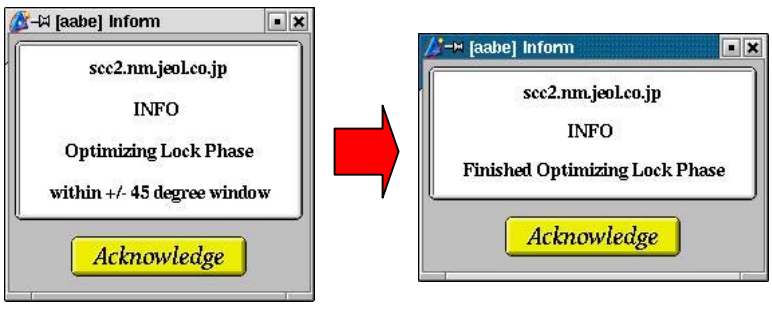
If the solvent does not appear in the list box, move the slider at the right side of the box.

2. Click on the button (☞④ in Fig.1.9).

When the NMR lock operates, the messages **LOCK ON** and **IDLE** are displayed at the bottom right of the **Lock Control** section.

3. Click on the button.(☞⑤ in Fig.1.9).

When the following message window appears, optimization of the Lock Phase will be performed.



Optimization started　　Optimization finished

■ Automatic resolution adjustment

◆ Specify the axes for automatic resolution adjustment(☞⑤ in Fig.1.9).

Select Z1 Z2 from the pulldown menu. When selection is complete, resolution adjustment for Z1 and Z2 axes starts automatically.

2

ONE-BUTTON MEASUREMENT

Chapter 2 explains automatic measurement using one-button operation.

2.1 GENERAL 2-1
2.2 STARTING AND ENDING MEASUREMENT 2-3
2.3 CANCELING MEASUREMENT 2-6
2.4 PRECAUTIONS 2-7

2.1 GENERAL

Automatic measurement which can be performed by simply clicking one button is called one-button measurement. When one-button measurement is performed, a series of conditions for sample settings, measurement, processing, and plotting, and their combinations are called methods. The following methods are displayed in the **Automation** window.

Table 2.1 Preset methods and measurements

Method	Measurement	Sequence name
Proton	1D ^{1}H normal measurement	single_pulse.ex2
Presaturation	1D ^{1}H normal measurement	single_pulse.ex2
	1D homo gated decoupling (Automatic solvent-elimination method)	single_pulse.ex2
Carbon	1D ^{13}C normal measurement	single_pulse_dec.ex2
Proton_and_Carbon	1D ^{1}H normal measurement	single_pulse.ex2
	1D ^{13}C normal measurement	single_pulse_dec.ex2
Carbon_and_DEPT_135	1D ^{13}C normal measurement	single_pulse_dec.ex2
	Automatic determination of ^{13}C atomic group by means of DEPT	dept.ex2
Carbon_and_APT	1D ^{13}C normal measurement	single_pulse_dec.ex2
	APT	apt.ex2
Edited_DEPT	1D ^{13}C normal measurement	single_pulse_dec.ex2
	Automatic determination of ^{13}C atomic group by means of DEPT	dept.ex2
Proton_and_COSY	1D ^{1}H normal measurement	single_pulse.ex2
	Homonuclear 2D ^{1}H-^{1}H COSY	cosy.ex2
Proton_and_DQF_COSY	1D ^{1}H normal measurement	single_pulse.ex2
	^{1}H double quantum filter COSY	dqf_cosy.ex2
Proton_and_NOESY	1D ^{1}H normal measurement	single_pulse.ex2
	^{1}H NOE correlation measurement	noesy.ex2
Proton_and_TOCSY	1D ^{1}H normal measurement	single_pulse.ex2
	TOCSY (TOtal Correlation SpectroscopY)	tocsy.ex2
Hetcor	1D ^{1}H normal measurement	single_pulse.ex2
	1D ^{13}C normal measurement	single_pulse_dec.ex2
	Heteronuclear 2D ^{1}H-^{13}C COSY	hector.ex2
Flock	1D ^{1}H normal measurement	single_pulse.ex2
	1D ^{13}C normal measurement	single_pulse_dec.ex2
	Flock	flock.ex2

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Method	Measurement	Sequence name
Combination_1	1D ^{1}H normal measurement	single_pulse.ex2
	1D ^{13}C normal measurement	single_pulse_dec.ex2
	Automatic determination of ^{13}C atomic group by means of DEPT	dept.ex2
	Homonuclear 2D ^{1}H-^{1}H COSY	cosy.ex2
	Heteronuclear 2D ^{13}C –^{1}H COSY	hector.ex2
Gradient_COSY	1D ^{1}H normal measurement	single_pulse.ex2
	Homonuclear 2D ^{1}H-^{1}H COSY	cosy_pfg.ex2
Gradient_DQF_COSY	1D ^{1}H normal measurement	single_pulse.ex2
	^{1}H double quantum filter COSY	dqf_cosy_pfg.ex2
Gradient_TOCSY	1D ^{1}H normal measurement	single_pulse.ex2
	TOCSY	tocsy_pfg.ex2
Gradient_PS_NOESY	1D ^{1}H normal measurement	single_pulse.ex2
	^{1}H homonuclear NOE correlation	noesy_pfgzz_pn.ex2
Gradient_HMQC	1D ^{1}H normal measurement	single_pulse.ex2
	1D ^{13}C normal measurement	single_pulse_dec.ex2
	^{1}H observation heteronuclear correlation	hmqc_pfg.ex2
Gradient_HMQC_with_y_proj	1D ^{1}H normal measurement	single_pulse.ex2
	^{1}H observation heteronuclear correlation spectroscopy	hmqc_pfg.ex2
Gradient_HMBC	1D ^{1}H normal measurement	single_pulse.ex2
	1D ^{13}C normal measurement	single_pulse_dec.ex2
	^{1}H observation heteronuclear long range correlation spectroscopy	hmbc_pfg.ex2
Gradient_HMBC_with_y_proj	1D ^{1}H normal measurement	single_pulse.ex2
	^{1}H observation heteronuclear long range correlation spectroscopy	hmbc_pfg.ex2
Gradient_HMQC_TOCSY	1D ^{1}H normal measurement	single_pulse.ex2
	1D ^{13}C normal measurement	single_pulse_dec.ex2
	HMQC-TOCSY	hmqc_tocsy_pfg.ex2
HMQC_TOCSY_with_y_proj	1D ^{1}H normal measurement	single_pulse.ex2
	HMQC-TOCSY	hmqc_tocsy_pfg.ex2
Combination_2	1D ^{1}H normal measurement	single_pulse.ex2
	1D ^{13}C normal measurement	single_pulse_dec.ex2
	Homonuclear 2D ^{1}H-^{1}H COSY	cosy_pfg.ex2
	^{1}H observation heteronuclear correlation spectroscopy	hmqc_pfg.ex2

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2.2 STARTING AND ENDING MEASUREMENT

■ Preparation for one-button measurement

● Setting the sample in the SCM

☞ Insert the sample, according to the procedure in Section1.3, “Sample preparation.”

● Opening the Automation window

◆ Click on the **Auto** button in the **Spectrometer Control** window.
The **Automation** window opens.

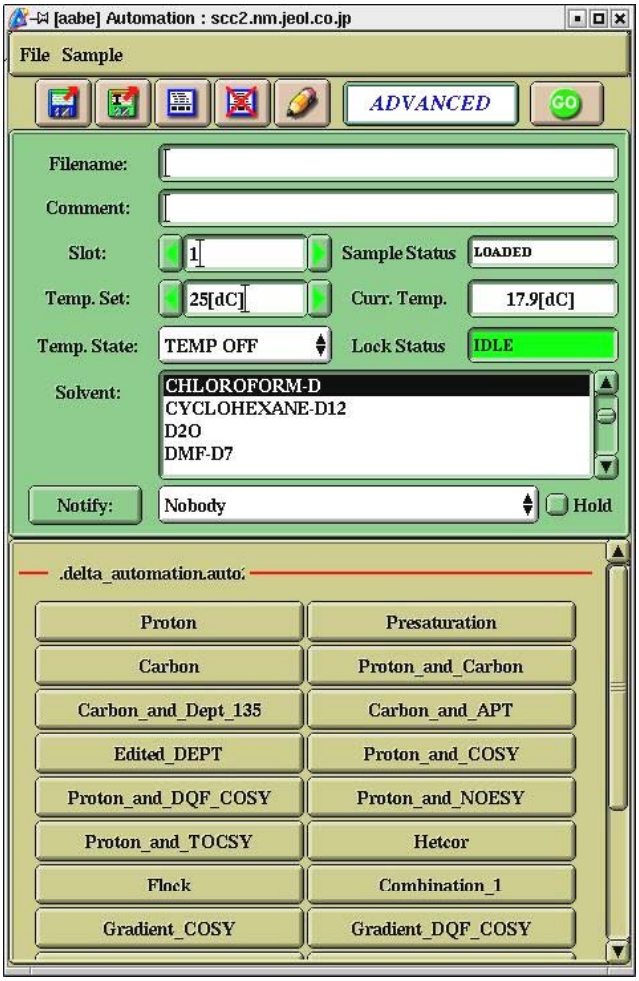

Fig. 2.1 Automation window

Filename	Usually, the name of the sample is used.
Comment	Enter a comment.
Slot	Sample number of the automatic sample changer
Sample Status	Messages about the present **s**ample status such as LOADED and EJECT
Temp. Set	**S**et temperature used during temperature control
Curr. Temp.	Present sample temperature

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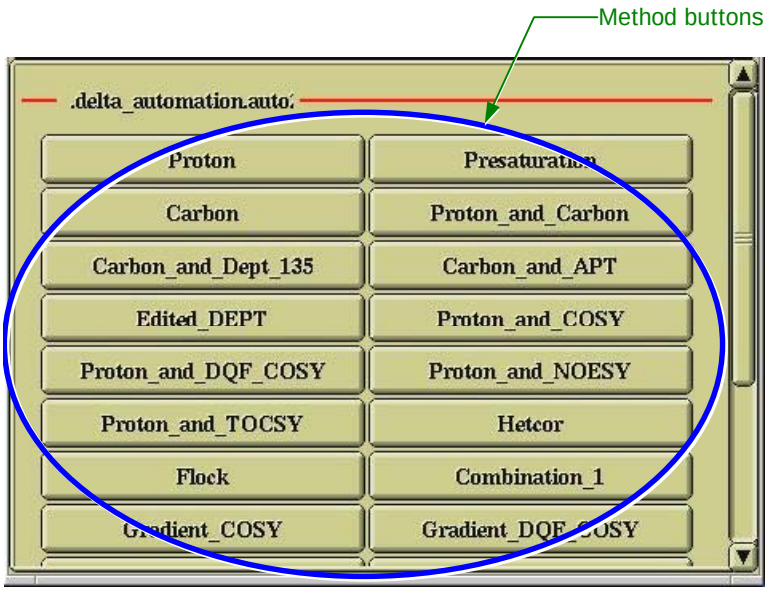
Temp. State	Specify whether or not to carry out temperature control using the temperature controller.
Lock Status	Present status of the NMR lock
Solvent	Select the sample solvent.
Notify	Information is sent to the specified E-mail address when measurement is complete. In order to use this function, it is necessary to perform the basic setting before using mail.
Hold	Even when a sample number is changed, Notify E-mail address is placed on hold.

Starting one-button measurement

◆ Click on the desired method button.

Measurement starts.



When measurement starts, the **Auto Queue** window opens as shown in Fig. 2.2.

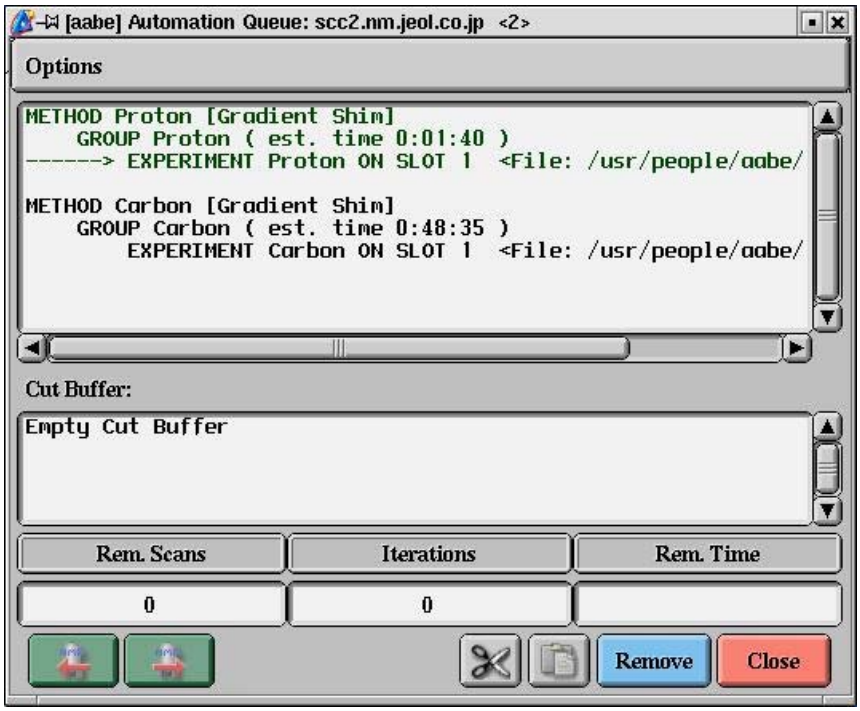


Fig. 2.2 Auto Queue window

■ Ending one-button measurement

After one-button measurement ends, remove the sample according to the following procedure.

1. Using the **Auto Queue** window, make sure that the one-button measurement has completed.
   If the method name has disappeared from the **Auto Queue** window, the one-button measurement is complete.
2. Open the **Sample** window.
3. Click on button.
   The sample will be ejected from the SCM. Make sure that the **Sample State** display changes to the eject condition.
4. Remove the sample from the SCM insertion port.

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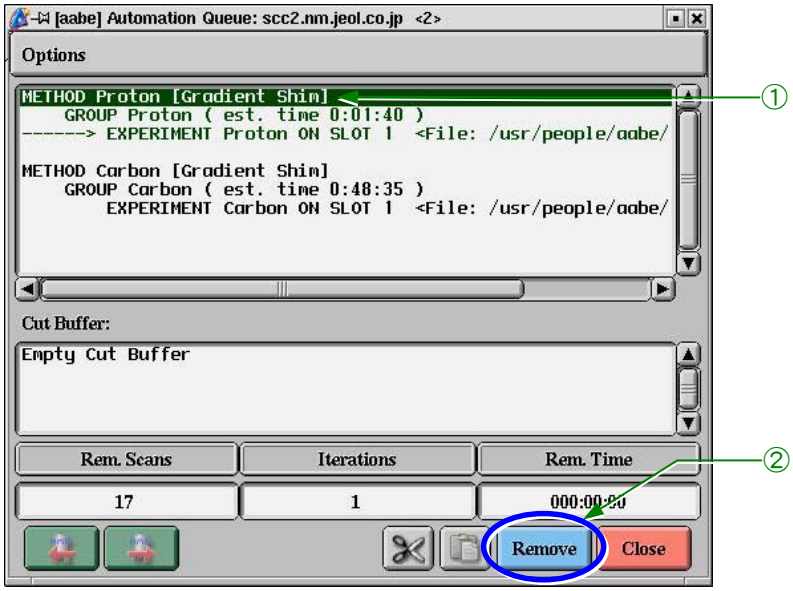
2.3 CANCELING MEASUREMENT

To cancel the measurement during one-button measurement, operate as follows.



✍ The numbers ① and ② are referred to in the following steps.

1. Click on the **Method** part of one button measurement that you want to chancel in the **Auto Queue** window (☞① in above figure).

The method is highlighted.

✍ Be sure to click on a **METHOD** without clicking on **GROUP** and **EXPERIMENT**.

2. Click on the **Remove** button (☞② in above figure).

☞ If you click on the **Remove** button when **GROUP** and **EXPERIMENT** are selected by mistake, cancellation is not performed correctly. Perform the cancellation operation again after updating the queue by selecting **Option**, the **Refresh Queue** in the menu bar.

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2.4 PRECAUTIONS

- **Specifying an NMR lock solvent**

  The difficulties which occurs most frequently in one-button measurements is an NMR lock error.
  To prevent NMR lock errors, make sure that the solvent name is entered correctly.

- **Automatic resolution adjustment**

  If the volumes of the samples to be measured are greatly different, or solid substances are present in the sample, the automatic resolution adjustment takes a long time.
  Under these conditions, the appropriate resolution may not be achieved.
  To prevent these difficulties, prepare the samples with about the same height of 4 cm, and align the bottom of the sample tube with that of the sample gauge.

- **Probe tuning**

  The probe tuning varies, depending on measurement parameters such as solvent or temperature. Especially, before performing a measurement such as DEPT that is sensitive to pulse width or when measuring a small amount of a sample that requires improvement of the S/N ratio, be sure to tune the probe.

- **Measurement conditions**

  The measurement conditions for general organic-compound samples are used for one-button measurement. If you want to measure the sample under special conditions, perform the measurement using individual operations.

- **Hard-disk capacity and data filename**

  Make sure that there is free space to save data before performing one-button measurement. The results of one-button measurement are saved in a file with a specified file name to which the method name is added. If the filename already exists, a new file with the version number one higher will be created.

- **Processing condition**

  In one-button measurement, parameters for data processing are prespecified. If you want to perform your own specific data processing, perform it later using the data that has been saved in the file.

- **Plotting**

  In one-button measurement, data will be plotted automatically. Therefore, make sure that chart paper is set in the printer correctly, and that the printer is online, before starting one-button measurement.

3

1D NMR MEASUREMENT

Chapter 3 explains the procedures for the basic 1D NMR measurement in the order of measurement, data processing, and plotting. It is assumed that the Delta system has been connected to the spectrometer, and that the sample setup, sample loading, NMR lock, resolution adjustment and other operations prior to measurement have already been performed. If you are not ready to start measurement, prepare for measurement according to Chapter 1, "Preparations for measurement".

3.1 SETTING 1D NMR MEASUREMENT CONDITIONS 3-1
3.1.1 Setting ^{1}H Measurement Conditions 3-1
3.1.2 Setting ^{13}C Measurement Conditions 3-4
3.2 STARTING AND ENDING MEASUREMENT 3-6
3.3 1D NMR DATA PROCESSING 3-7
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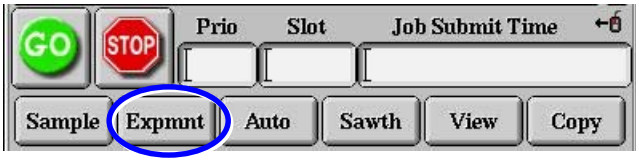
3.1 SETTING 1D NMR MEASUREMENT CONDITIONS

3.1.1 Setting ^{1}H Measurement Conditions

1. Click on the **Expmnt** button in the **Spectrometer Control** window.



The **Open Experiment** window opens.

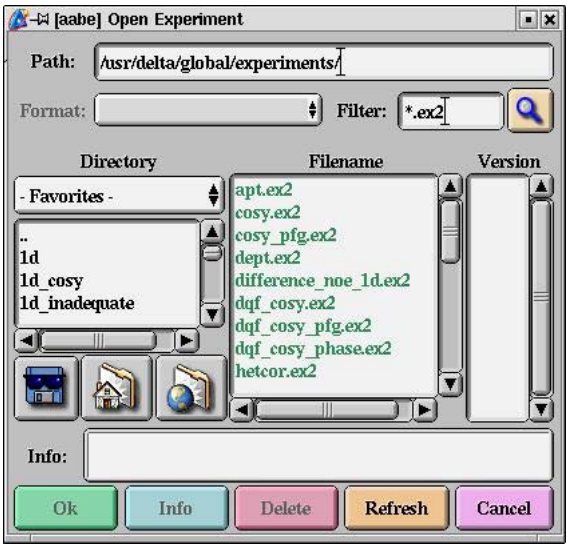


Fig. 3.1 Open Experiment window

2. Click on the button in the **Open Experiment** window.
A list of the Experiment files[*1] in the Global directory [*2] is displayed.

3. Select the measurement mode **single_pulse.ex2** from the **Open Experiment** window, and click on the **Ok** button.
The **Experiment Tool** window (Fig. 3.2) opens. This **Experiment Tool** window consists of the four sections **Header**, **Instrument**, **Acquisition**, and **Pulse.**

---

*1 The Experiment files contain the measurement modes, standard measurement conditions, and steps for processing data. The file type is **.ex2.**
*2 The Global directory is the directory in which the standard files supplied from JEOL are stored. The files in this directory cannot be changed.

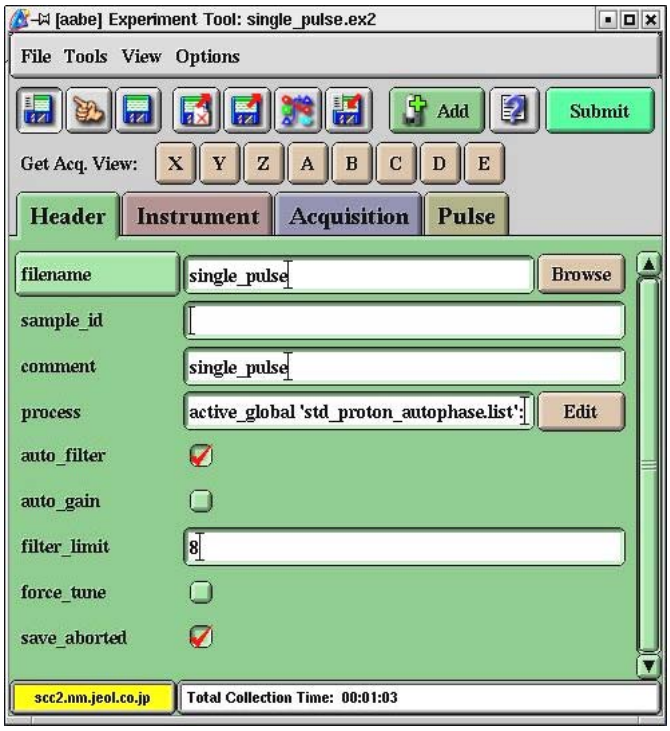


Fig. 3.2 Experiment Tool window

4. Set the necessary parameters.

The following parameters are usually used.

☞ For information about the other parameters, refer to the separate volume, "USER'S MANUAL, MEASUREMENT".

✍ Parameters can be displayed by double-clicking on **Header**, **Instrument**, **Acquisition** or **Pulse**.

sample_id	Name to identify sample
comment	**C**omment on measurement data
auto_gain	If you want the instrument to adjust the receiver gain automatically, click on the button to mark it with a check mark. The results that were acquired using the automatic gain will be displayed on the ***Master Console*** window and the **Spectrometer Control** window.
solvent	Solvent used for NMR lock. If the NMR lock was already used on the ***Sample*** window or another window, the solvent used has already been set.
recvr_gain	Receiver gain, if automatic gain is not selected.
x_points	Number of data points to measure in each scan
scans	Number of scans to accumulate

5. Make sure that other necessary parameters are set appropriately.

✍ Parameters can be displayed by double-clicking on **Header**, **Instrument**, **Acquisition** or **Pulse**.

x_domain	Observation nucleus: Proton

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x_offset	Observation center frequency: 5 ppm
x_sweep	**O**bservation range: 15 ppm
total_time	**A**pproximate time necessary for measurement
x_pulse	Pulse width to be used for measurement
relaxation_delay	Pulse delay time

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3.1.2 Setting ^{13}C Measurement Conditions

1. Click on the **Expmnt** button in the **Spectrometer Control** window.
The **Open Experiment** window opens.

2. Click on the button in the **Open Experiment** window.
A list of the Experiment files in the Global directory is displayed.

3. Select the measurement mode **single_pulse_dec.ex2** from the **Open Experiment** window, and click on the **Ok** button.
The **Experiment Tool** window opens.

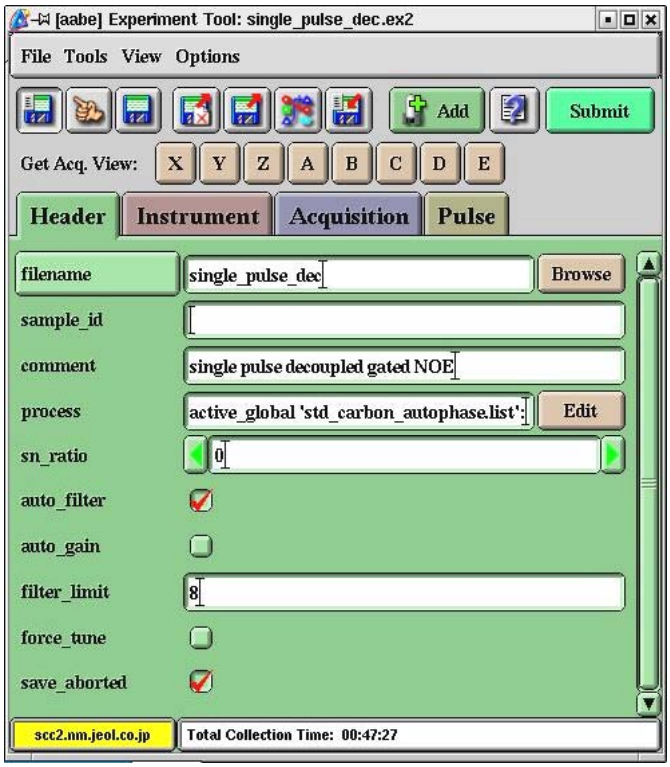

Fig. 3.3 Experiment Tool window

4. Set the necessary parameters.
The following parameters are usually used.

☞ For information about the other parameters, refer to the separate volume, "USER'S MANUAL , MEASUREMENT".

✍ Parameters can be displayed by double-clicking on **Header**, **Instrument**, **Acquisition** or **Pulse**.

sample_id	Name to identify sample
comment	**C**omment on measurement data
auto_gain	If you want the instrument to adjust the receiver gain automatically, click on the button to mark it with a check mark.

solvent	Solvent used for NMR lock. If the NMR lock was already used on the **Sample** window or another window, the used solvent has been set.
recvr_gain	Receiver gain, if automatic gain is not selected.
irr_noise	**N**oise source for irradiation. Normally, **WALTZ** is used**.**
x_points	Number of data points to measure in each scan
scans	Number of scans to accumulate
irr_domain	Irradiation nucleus: Proton
irr_offset	Irradiation position.

5. Make sure that other necessary parameters are set appropriately.

Parameters can be displayed by double-clicking on **Header**, **Instrument**, **Acquisition** or **Pulse**.

x_domain	Observation nucleus: Carbon13
x_offset	Observation center frequency: 100 ppm.
x_sweep	**O**bservation range: 250 ppm
total_time	**A**pproximate time necessary for measurement
x_pulse	Pulse width to be used for measurement
relaxation_delay	Pulse delay time.

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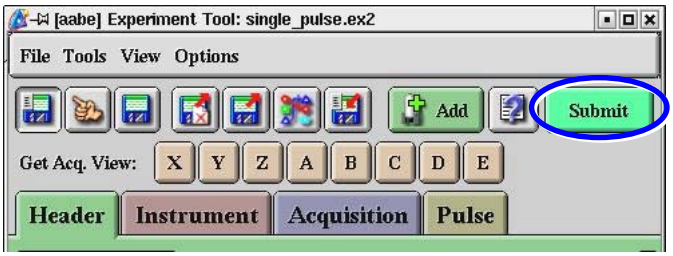
3.2 STARTING AND ENDING MEASUREMENT

This section explains how to start and end 1D NMR measurement and how to confirm the measurement status.

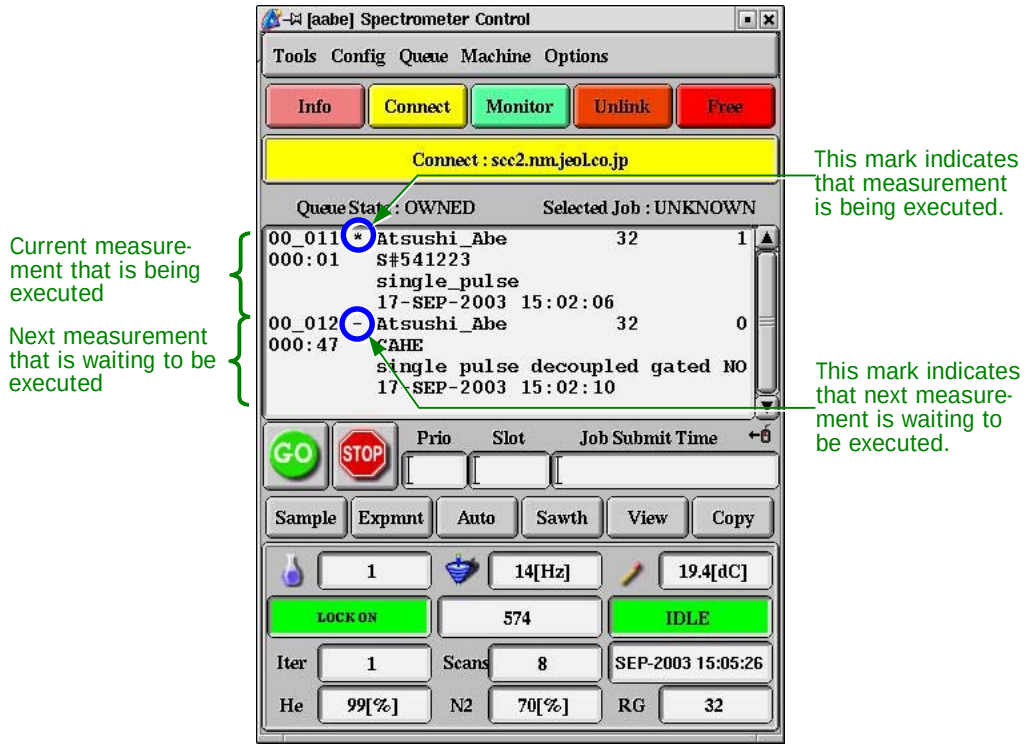
■ Starting measurement and displaying the status

◆ Click on the **Submit** button in the **Experiment Tool** window.

The measurement is entered into the spectrometer-control computer's queue. The spectrometer executes measurement on a first-in, first-out basis.



Commands for starting measurements can be issued repeatedly, even if another measurement is being performed. After one measurement finishes, the next measurement will be started under the stored measurement conditions.



■ Ending measurement

When the measurement finishes, the data processing window opens.

☞ To stop the measurement during operation, refer to Chapter 5, "Queuing".

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3.3 1D NMR DATA PROCESSING

After measurement is complete, data is automatically forwarded from the spectrometer, and the following processing is automatically executed.

- Correction of the DC components of FID (Free Induction Decay)
- Multiplication by window functions
- FFT (Fast Fourier Transformation)
- Automatic phase correction

This section explains data processing following phase correction.
When measurement is completed, the following **1D Processor** window opens.

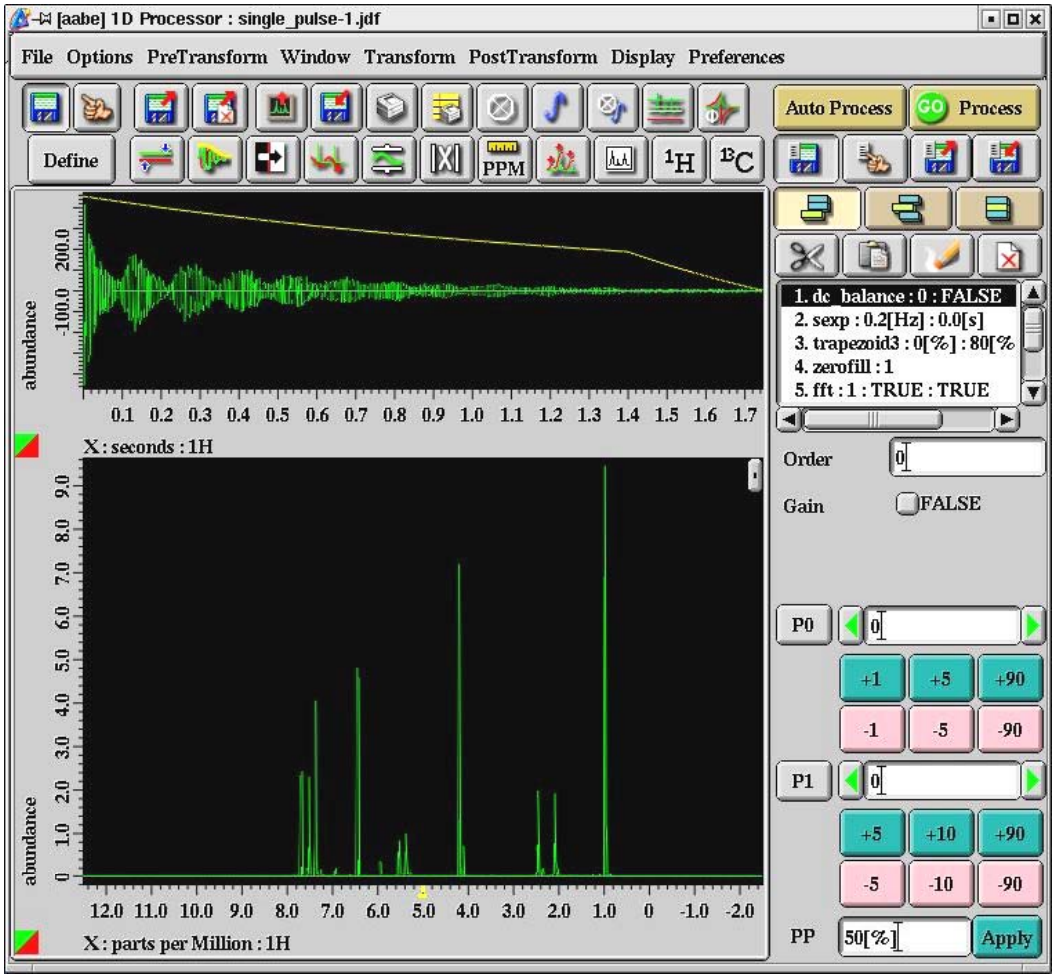

Fig. 3.4 1D Processor window

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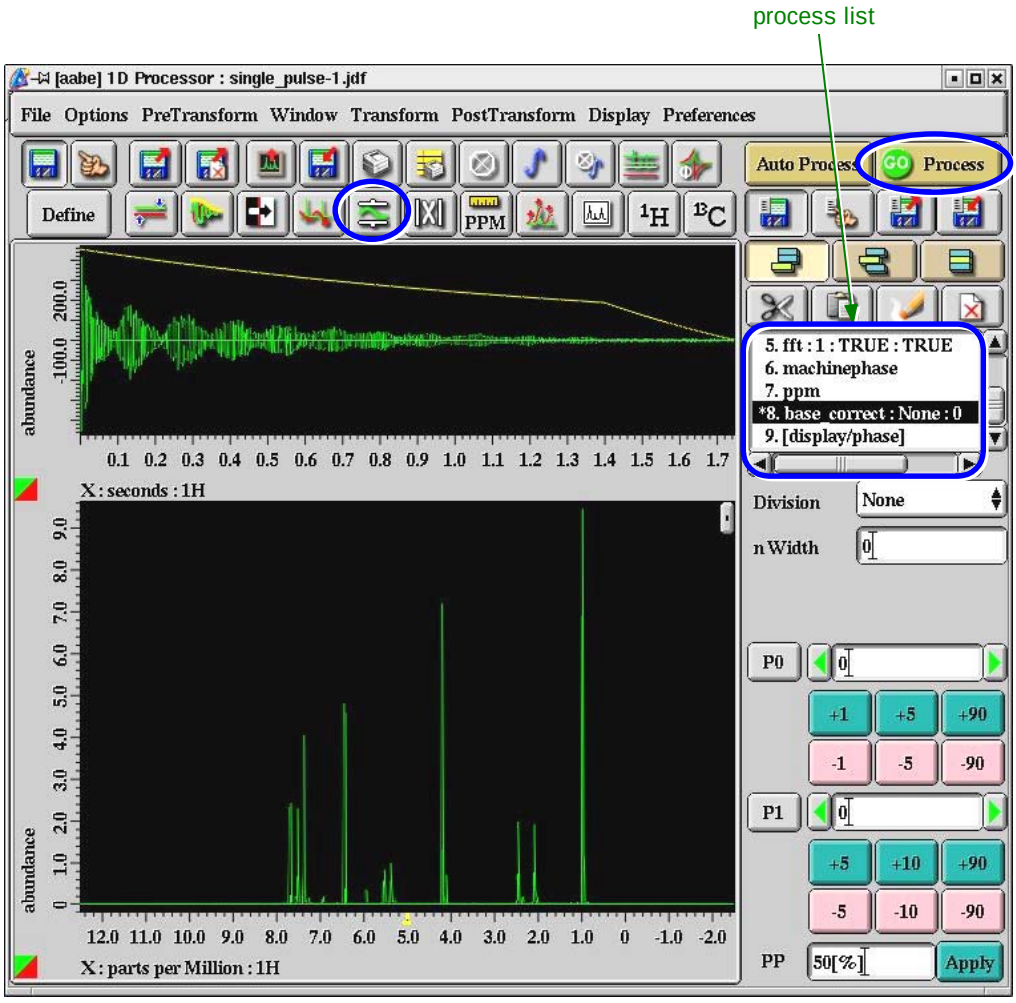
3.3.1 Automatic Baseline Correction

1. Click on the button in the **1D Processor** window.
An item, **Base Correct,** is added to the process list.

2. Click on the **Process** button.
The spectrum with the baseline corrected is displayed in the lower spectral display area.



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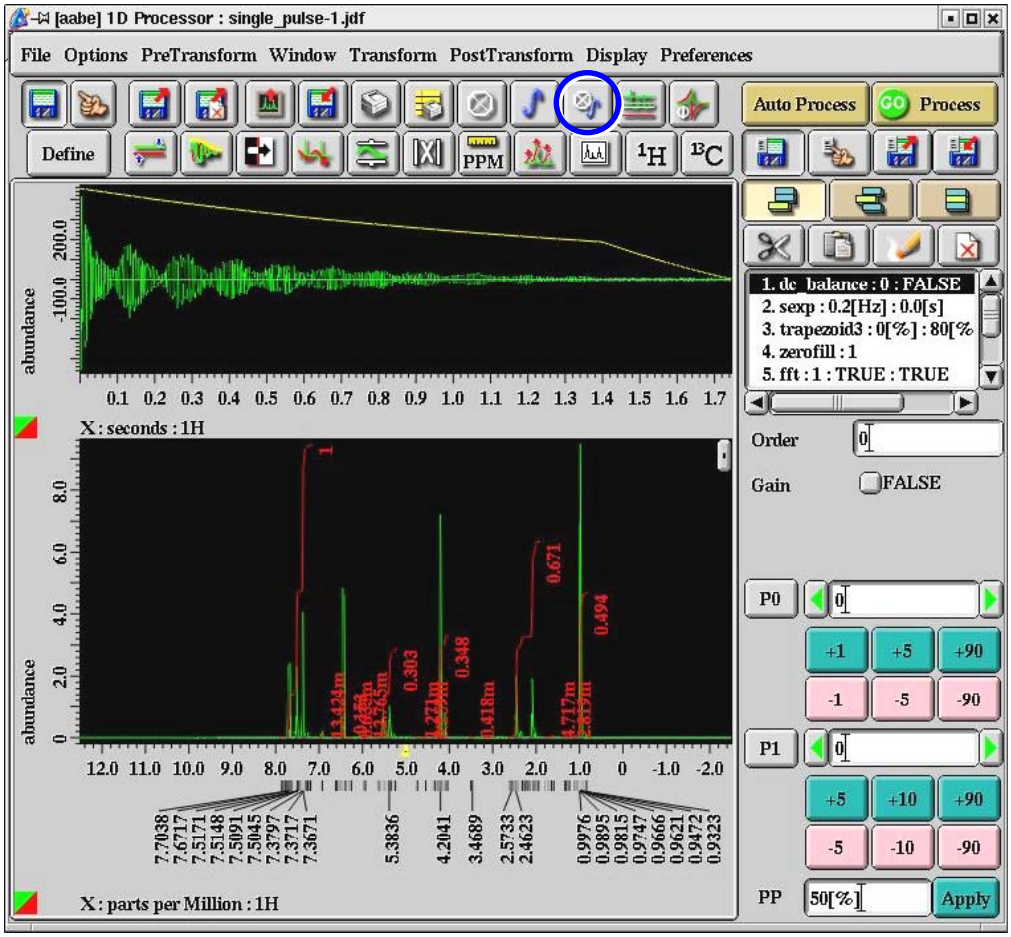
3.3.2 Automatic Peak Detection and Automatic Integration

◆ Click on the button in the **1D Processor** window.

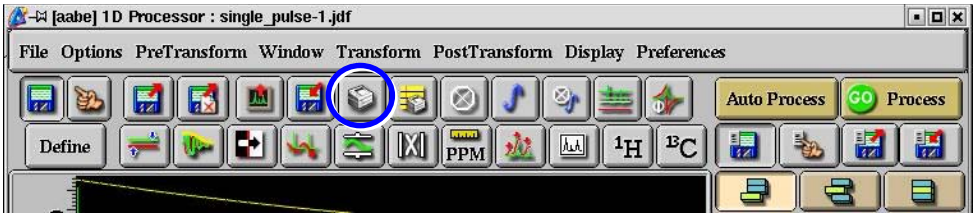
Automatic peak detection and automatic integration are carried out, and the results are displayed in the lower spectral display area in the **1D Processor** window.



3.3.3 Plotting

The standard method of plotting is as follows.

◆ Click on the button in the **1D Processor** window.



The processed spectrum in the lower display area is plotted on paper.

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3.3.4 Changing the Display Range

■ Usage of Cursor Tool bar

The Cursor Tool bar is used to expand or reduce spectra. The Cursor Tool bar is available in each display area.

This section explains basic usage of the Cursor Tool bar.

● To display the Cursor Tool bar

◆ Move the mouse pointer to the spectral display area in which you want to display the Cursor Tool bar.

The Cursor Tool bar is displayed at the upper right in the spectral display area.

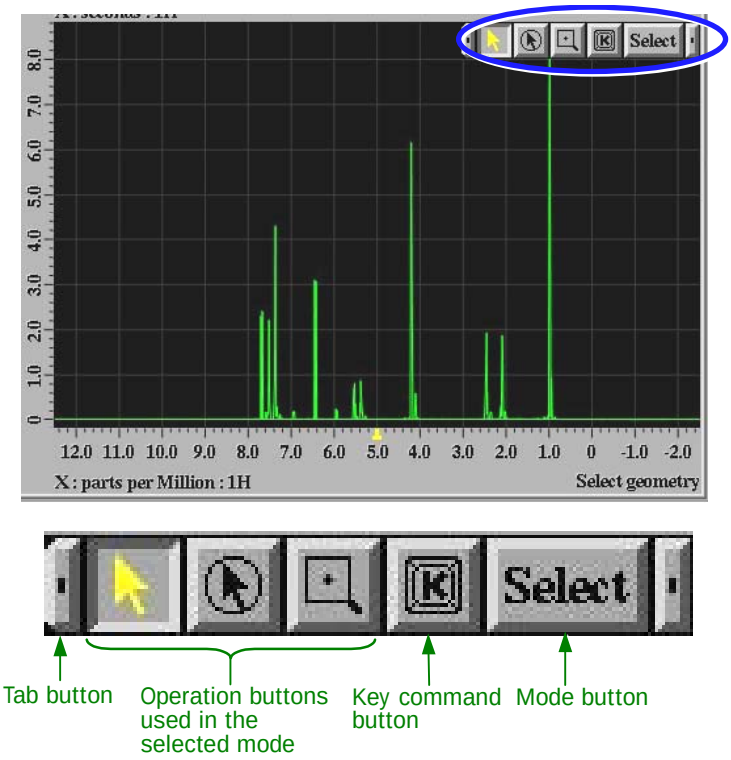

Fig. 3.5 Normal display of Cursor Tool bar

● To minimize the Cursor Tool bar

◆ Click on the tab button.

The Cursor Tool bar changes from the normal display shown in Fig 3.5 to the minimized display shown in Fig 3.6.

Fig. 3.6 Minimized Cursor Tool bar

● To return the minimized Cursor Tool bar to the normal display

◆ Click on the tab button.

The minimized Cursor Tool bar returns to the normal display shown in Fig 3.5.

To switch the Cursor Tool mode

1. Move the mouse pointer to the mode button at the right end of the Cursor Tool bar; then press and hold the left mouse button.

The following thirteen modes are displayed under the mode button.

Zoom	To expand, reduce, or move spectra.
Select	To select data or a geometry.
Region	To display a selected region in another geometry.
Cursor	To correct the baseline, or to display the difference between two points
Reference	To set a chemical shift reference axis marker.
Peak	To execute a peak pick.
Pick	To set the slice position of 2D data or read peak positions.
Integral	To perform integration.
Annotation	To display an annotation in the geometry.
PIP	To display a selected part of the geometry within the present geometry.
Phase	To adjust the phase.
Molecule	To display a structural formula and molecular formula in the geometry.
Measure	Measure distance between peaks

☞ This chapter explains only the **Zoom** mode. For more information about the other modes, refer to the separate volume, “USER'S MANUAL, DATA PROCESSING”.

2. Move the mouse pointer with the left mouse button still pressed to the mode you want to select, and release the mouse button.

The Cursor Tool bar changes to the buttons for the selected mode.

To select a button

◆ Click on the button you want.

The button you clicked on changes to appear selected or pressed. The explanation of the selected button is also displayed at the bottom right of the spectral display area.

☞ Clicking the middle mouse button on the mode button with displays a list of the buttons which can be used in the currently selected mode and an explanation of these buttons. You can select the button you want to use from the list.

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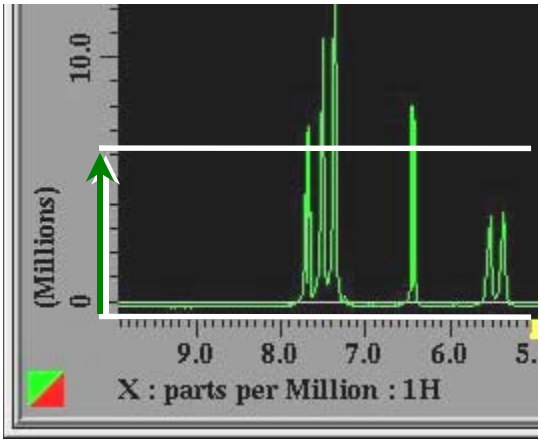
Expanding and resetting spectra in the 1D Processor window

To expand a spectrum vertically

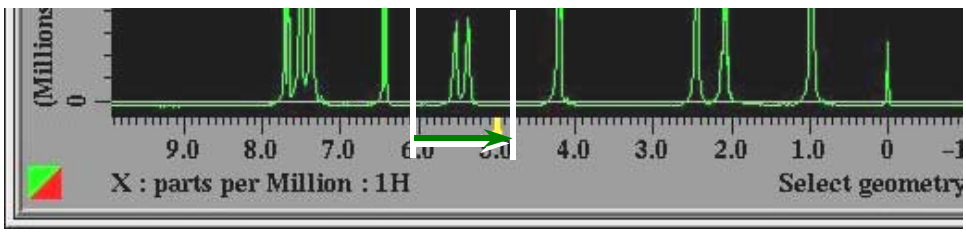
1. Select the **Zoom** mode from the Cursor Tool bar or press the F1 key on the keyboard.
   The Cursor Tool mode becomes **Zoom,** and the mouse pointer on the spectral screen changes to .
2. Move the mouse pointer to the position that will become the upper end of the expanded Y-axis.
3. Drag the left mouse button to the position that will become the lower end of the expanded Y-axis.
4. Release the left mouse button.



The spectrum is expanded vertically.

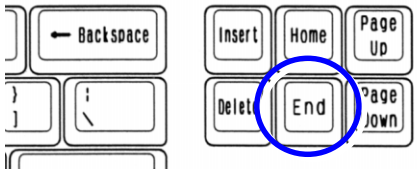
To expand a spectrum horizontally

1. Select the **Zoom** mode from the Cursor Tool bar or press the F1 key on the keyboard.
   The Cursor Tool mode becomes **Zoom.**
2. Move the mouse pointer to the position that will become the left end of the expanded X-axis.
3. Drag the left mouse button to the position that will become the right end of the expanded X-axis.
4. Release the left mouse button.



The spectrum is expanded horizontally.

- **To adjust the display to the intensity of the highest peak displayed**
  - Press the End key on the keyboard.



The highest peak in the spectral region displayed at present is expanded or reduced to fit within the screen.

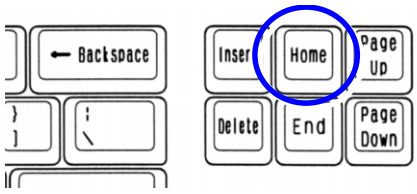
- **To return the spectrum display to its previous conditions**
  - Press the Backspace key on the keyboard to return to the previous conditions.

You can return to the previous conditions up to 16 times.

When you press the Backspace key, both vertical and horizontal expansions return to their previous values.
You cannot selectively return only the vertical or horizontal size to its previous value.

- **To return the spectrum display to its initial conditions**
  - Press the Home key on the keyboard.

All horizontal and vertical expansions return to their initial values.



4

2D NMR MEASUREMENT

Chapter 4 explains the procedures for the basic 2D NMR measurement in the order of measurement, data processing, and plotting. It is assumed that the Delta system has been connected to the spectrometer, and that the sample setup, sample loading, NMR lock, resolution adjustment and other preparations for measurement have already been performed. If you are not ready to start measurement, carry out the procedures in Chapter 1, “Preparation for measurement”.

4.1 SETTING 2D NMR MEASUREMENT CONDITIONS 4-1
4.1.1 HH COSY Measurement 4-1
4.1.2 HETCOR Measurement 4-4
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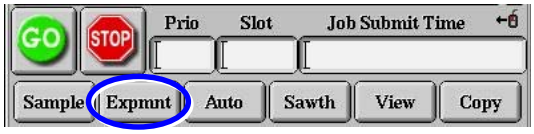
4.1 SETTING 2D NMR MEASUREMENT CONDITIONS

This section explains how to set the conditions for measuring ^{1}H–^{1}H homonuclear 2D NMR (HH COSY) and ^{13}C detection heteronuclear 2D NMR (HETCOR).

4.1.1 HH COSY Measurement

1. Click on the **Expmnt** button in the **Spectrometer Control** window.



The **Open Experiment** window opens.

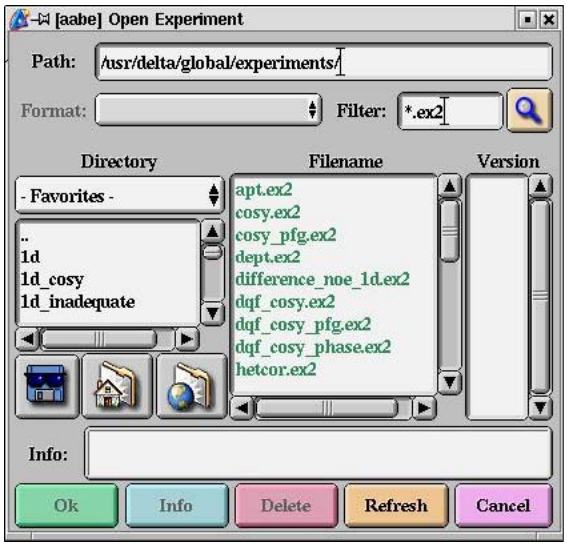


Fig. 4.1 Open Experiment window

2. Select the measurement mode **cosy.ex2** from the list displayed in the **Open Experiment** window, and click on the **Ok** button.

The **Experiment Tool** window opens.

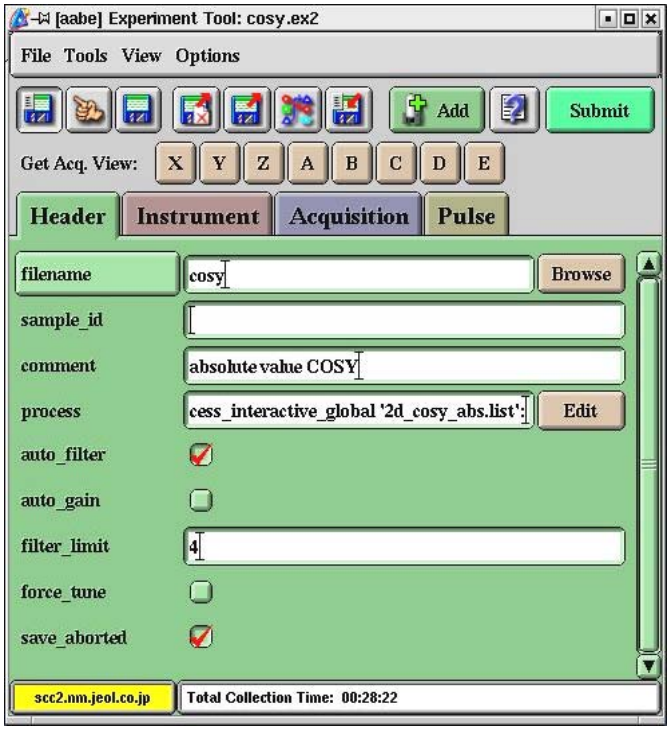


Fig. 4.2 Experiment Tool window

3. Set the necessary parameters.

The parameters which are usually used are explained below.

☞ For information about other parameters, refer to the separate MEASUREMENT user's manual.

✍ Parameters can be displayed by double-clicking on **Header**, **Instrument**, **Acquisition** or **Pulse**.

sample_id	Name to identify sample
comment	Comments on measurement data
auto_gain	Normally, do not check this box for 2D measurement.
solvent	Solvent used for an NMR lock
recvr_gain	Set the gain which was used for normal ^{1}H measurement.
x_points	Number of data points on the f_2 axis
scans	Number of scans to accumulate
y_points	Number of data points on the f_1 axis
pulse_angle_1	Flip angle. 90 [deg] in Cosy.
pulse_angle_2	Flip angle. 90 [deg] or 45 [deg] in Cosy.
relaxation_delay	Pulse delay time

4. Verify the necessary parameters.

✍ Parameters can be displayed by double-clicking on **Header**, **Instrument**, **Acquisition** or **Pulse**.

x_domain	Observation nucleus: Proton
x_offset	Observation center frequency (ppm)

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x_sweep	Observation range (ppm)
total_time	Approximate time necessary for measurement
x_90_width	90° pulse width
pulse_1	First pulse width to be used for measurement
pulse_2	Second Pulse width to be used for measurement

x_offset and **x_sweep** can be set from 1D NMR data which has already been processed. For the procedure, refer to Section 4.1.3, “Setting the measurement range from 1D NMR data.”

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4.1.2 HETCOR Measurement

1. Click on the **Expmnt** button in the **Spectrometer Control** window.
The **Open Experiment** window opens.

2. Select the measurement mode **htcor.ex2** from the list displayed in the **Open Experiment** window, and click on the **Ok** button.
The **Experiment Tool** window opens.

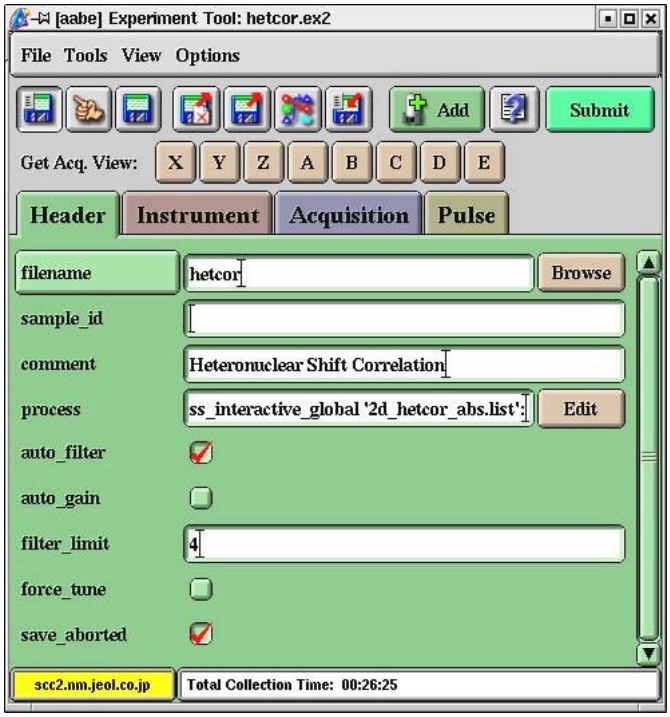

Fig. 4.3 Experiment Tool window

3. Set the necessary parameters.
The parameters which are usually used are explained below.

☞ For information about other parameters, refer to the separate MEASUREMENT user's manual.

✍ Parameters can be displayed by double-clicking on **Header**, **Instrument**, **Acquisition** or **Pulse**.

sample_id	Name to identify sample
comment	Comments on measurement data
auto_gain	Normally, do not check this box for 2D measurement.
solvent	Solvent used for NMR lock
recvr_gain	Set the gain which was used for ^{13}C 1D measurement.
x_points	Number of data points on the f_2 axis
scans	Number of scans to accumulate
y_points	Number of data points on the f_1 axis
j_constant	J value

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relaxation_delay	Pulse delay time

4. Verify the necessary parameters.

Parameters can be displayed by double-clicking on **Header**, **Instrument**, **Acquisition** or **Pulse**.

x_domain	Observation nucleus: Carbon
x_offset	Observation center frequency (ppm)
x_sweep	Observation range (ppm)
y_domain	Irradiation nucleus: Proton
y_offset	Irradiation center frequency (ppm)
y_sweep	Irradiation range (ppm)
total_time	Approximate time necessary for measurement
x_pulse	^{13}C pulse width to be used for measurement
y_pulse	^{1}H pulse width to be used for measurement

x_offset, x_sweep, y_offset, and **y_sweep** can be set from 1D NMR data which has already been processed. For the procedure, refer to Section 4.1.3, “Setting the measurement range from 1D NMR data.”

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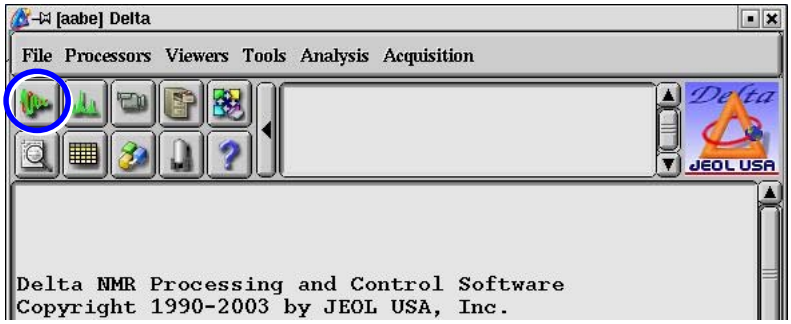
4.1.3 Setting the Measurement Range from 1D NMR Data

To measure ^{1}H-^{1}H homonuclear 2D NMR, ^{1}H 1D NMR data is necessary. To measure ^{1}H detection heteronuclear 2D NMR or ^{13}C detection heteronuclear 2D NMR, ^{1}H 1D data and ^{13}C 1D data are necessary. If 1D data is already loaded in the **1D Processor** window, proceed to ■ Setting the measurement range from 1D NMR data. If these 1D NMR data are not yet displayed in the **1D Processor** window, load data in the **1D Processor** window from the file as follows.

■ Loading 1D data

1. Click on the button in the **Delta Console** window.


[aabe] Delta
File Processors Viewers Tools Analysis Acquisition
JEOL USA
Delta NMR Processing and Control Software
Copyright 1990-2003 by JEOL USA, Inc.

The **Open Data for Processing** window opens.

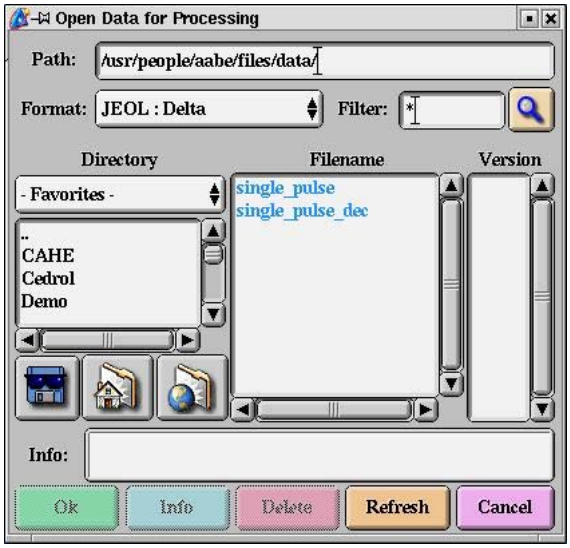


Fig. 4.4 Open Data for Processing window

2. Using the mouse, select the 1D NMR data from the data file list in the **Open Data for Processing** window.

3. After you select the file from the **Open Data for Processing** window, click on the **Ok** button.

The data is loaded, and the **1D Processor** window opens.

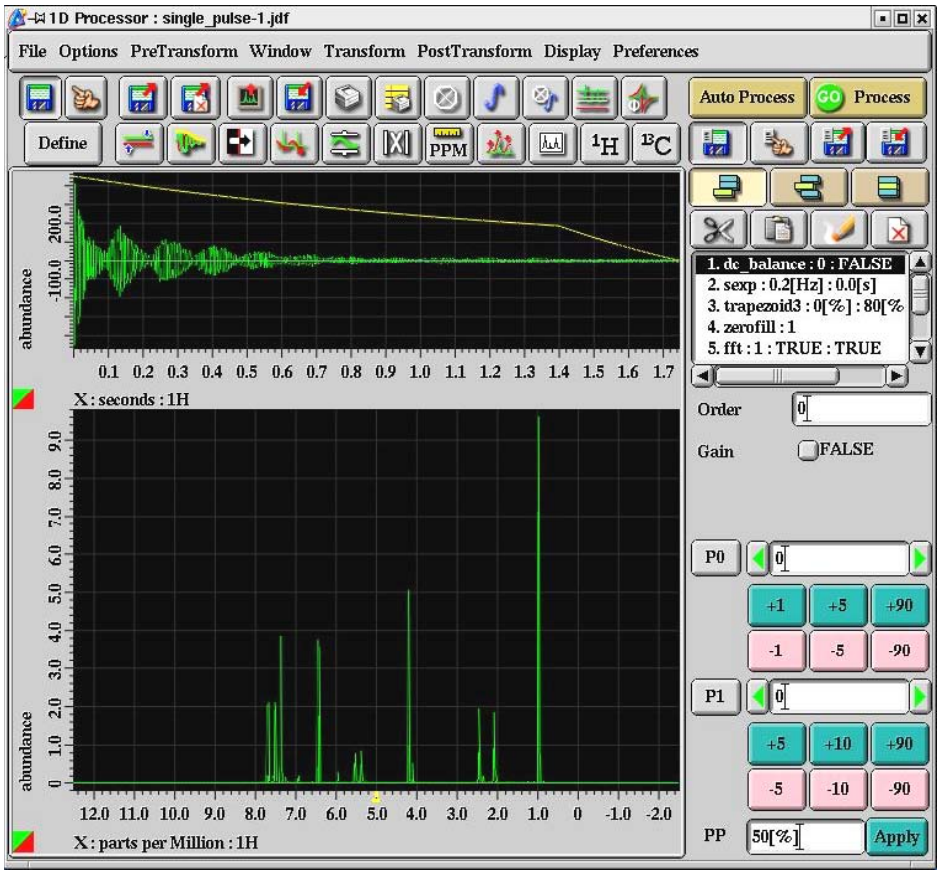


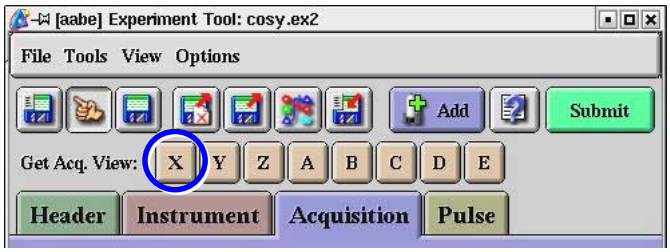
Fig. 4.5 1D Processor window

4. If the loaded 1D NMR data is FID, perform data processing such as FFT, phase correction, and reference setting, referring to Section 3.3 1D NMR data processing.

   If data processing has already been executed, proceed to the next step.

■ Setting the measurement range from 1D NMR data (HH COSY)

1. Expand the processed 1D NMR data to the range to be used for 2D NMR measurement.
2. Click on the button in the **Experiment Tool** window.
3. Click on the **View X** button.



The mouse pointer changes to .

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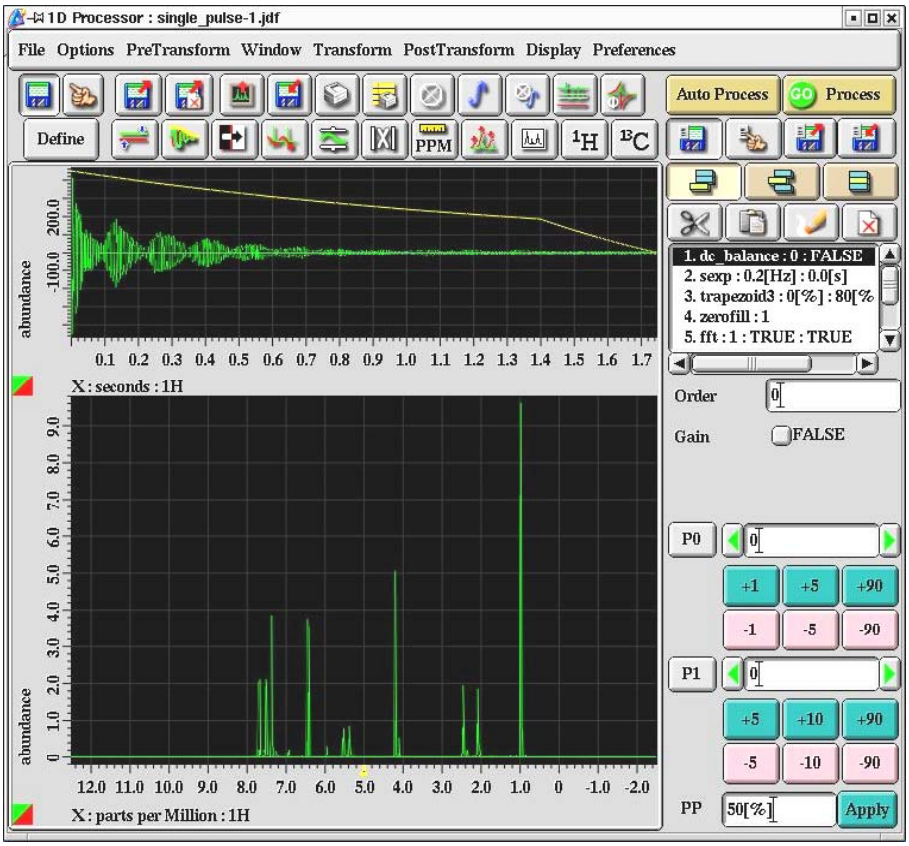
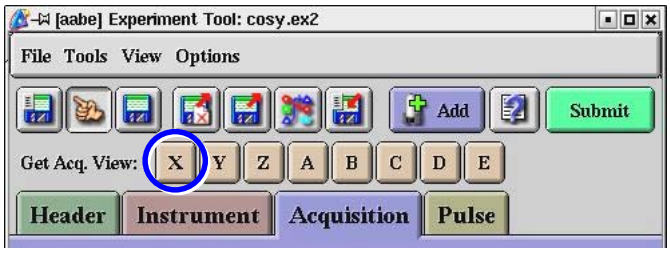
4. Move the mouse pointer to the position of the processed 1D data, and click the left mouse button.



x_offset and **x_sweep** are set to the offset and range values of the area where the 1D NMR data is displayed.

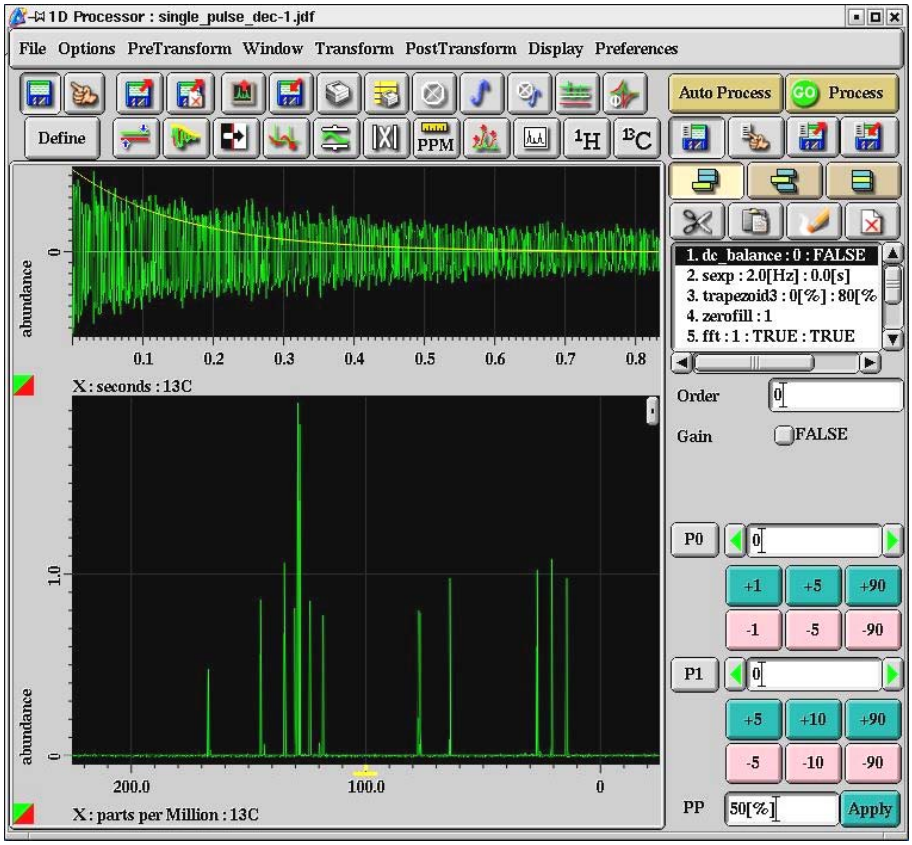
■ Setting the measurement range from 1D NMR data (HETCOR)

1. Expand the processed 1D NMR data to the range to be used for 2D NMR measurement.
2. Click on the button in the **Experiment Tool** window.
3. Click on the **View X** button.



The mouse pointer changes to .

4. Move the mouse pointer to the position of the processed 1D data (^{13}C 1D NMR data, for example), and click the left mouse button.



x_offset and **x_sweep** are set to the offset and range values of the area where the 1D NMR data is displayed.

5. Click on the **View Y** button as well.

The mouse pointer changes to the shape of a finger.

6. Move the mouse pointer to the position of the 1D data (^{1}H 1D data, for example), and click the left mouse button.

y_offset and **y_sweep** are set to the offset and range values of the area where the 1D NMR data is displayed.

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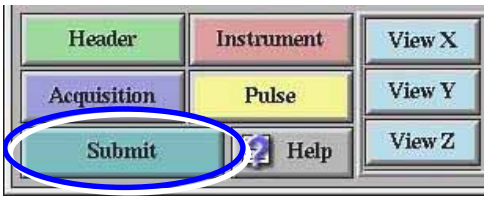
4.2 STARTING AND ENDING MEASUREMENT

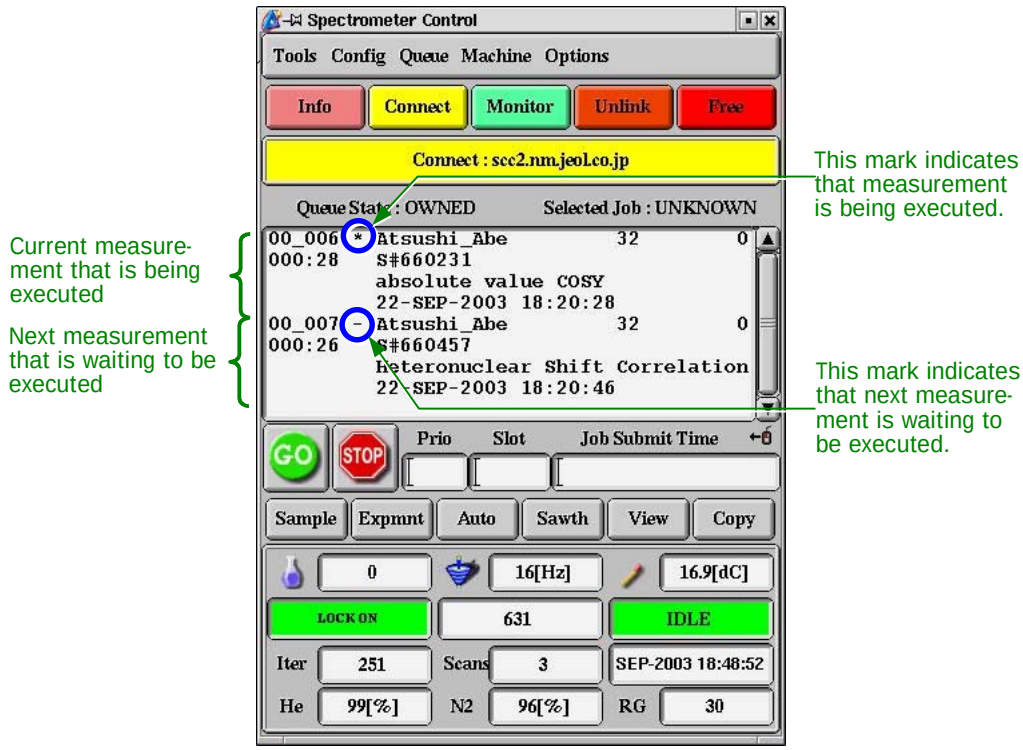
■ Starting measurement and displaying the present status

◆ Click on the **Submit** button in the **Experiment Tool** window.

The measurement is entered into the spectrometer-control computer's queue. The spectrometer executes measurement on a first-in, first-out basis.



The command for starting measurement can be issued repeatedly, even if another measurement is being performed. After one measurement finishes, the next measurement will be started under the stored measurement conditions.



■ Ending measurement

When the measurement finishes, the **nD processor** window opens.

☞ To stop the measurement during operation, refer to Chapter 5, "Queuing."

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4.3 DATA PROCESSING OF 2D NMR

This section explains data processing immediately after completion of NMR measurement.
When measurement is complete, Data will be sent from the spectrometer to the processing computer, and the **nD Processor** window will open.
Data will be processed according to the process list in the pulse sequence.

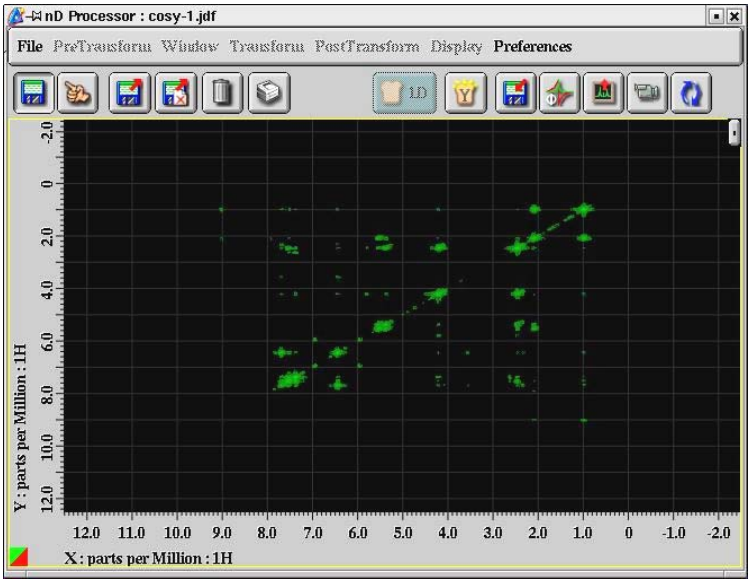
nD Processor : cosy-1.jdf
File PreTransform Window Transform PostTransform Display Preferences
1D
Y : parts per Million : 1H
X : parts per Million : 1H

Fig. 4.6 nD Processor window

If you change the processing conditions, click on the button to display the process list. If you click on the button again after changing the process list, processing will be executed again according to the changed contents.

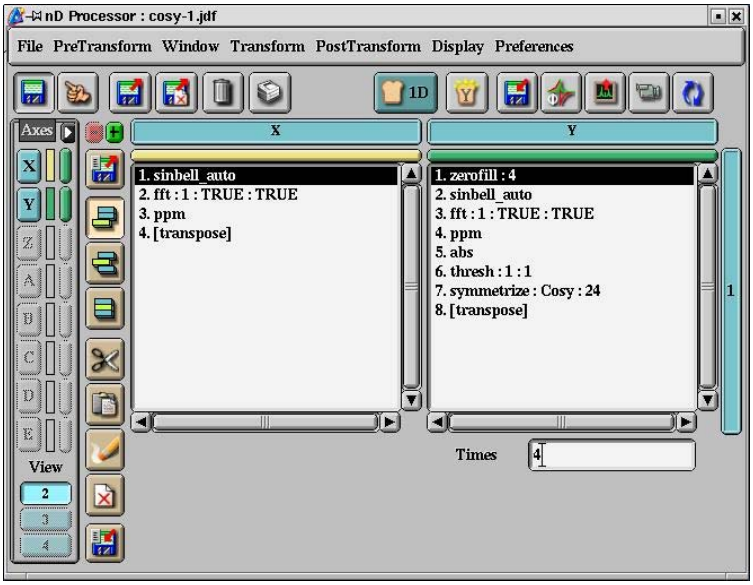

Fig. 4.7 nD Processor window (Process list display screen)

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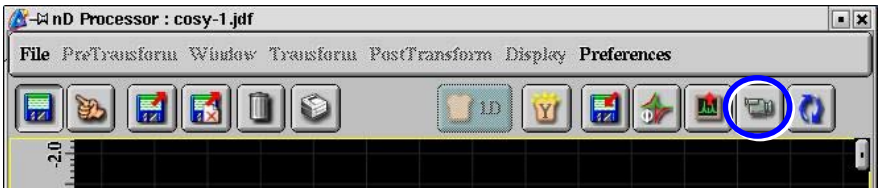
4.3.1 Displaying Data Using 2D Viewer

- Click on the button in the **nD Processor** window.



A new **2D Viewer** opens, and projection data other than 2D data are displayed.

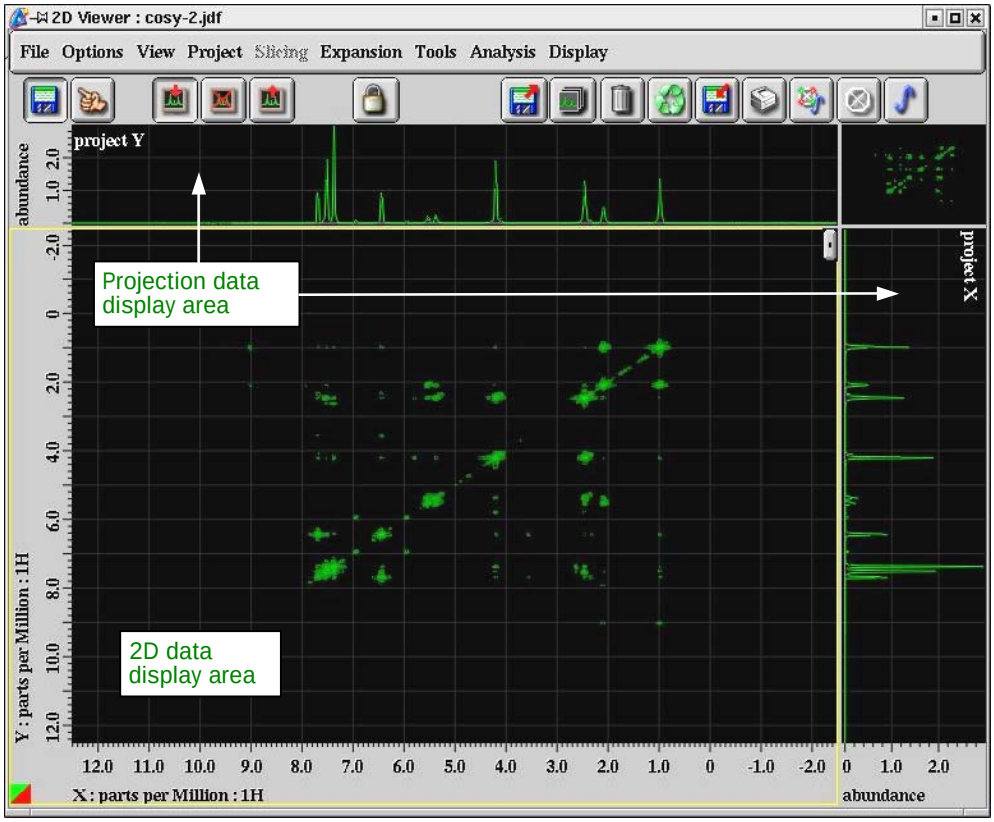
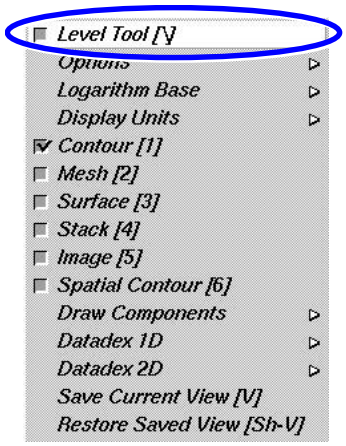

2D Viewer : cosy-2.jdf
File Options View Project Slicing Expansion Tools Analysis Display
project Y
abundance
Projection data display area
project X
2D data display area
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

Fig. 4.8 2D Viewer window

4.3.2 Setting the Conditions for Displaying Contour Lines

The ***2D Viewer*** window is used to set the levels of the contour lines.
The ***Level Tool*** window is used to change the levels of the contour lines.

1. Click the right mouse button to display the pop-up menu, and select **Level Tool.**



The **Level Tool** window opens.

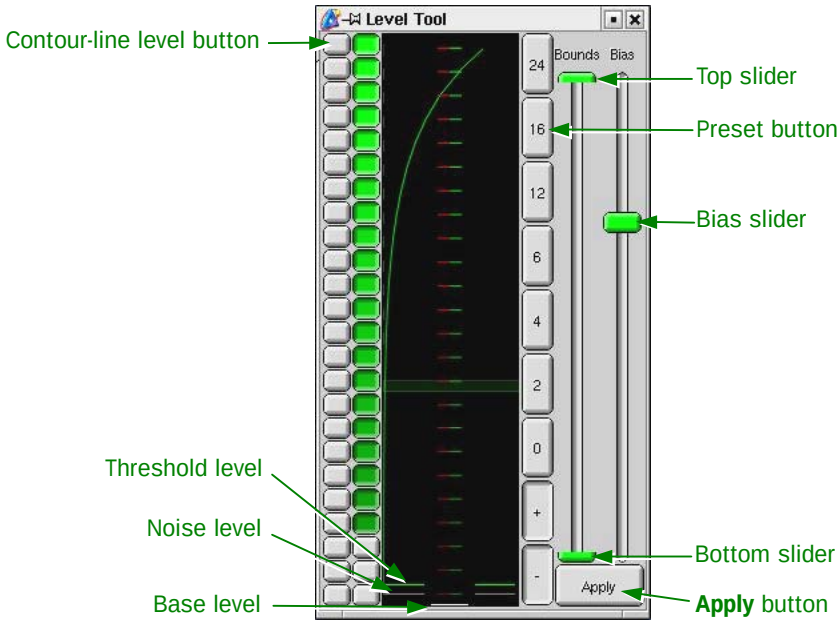


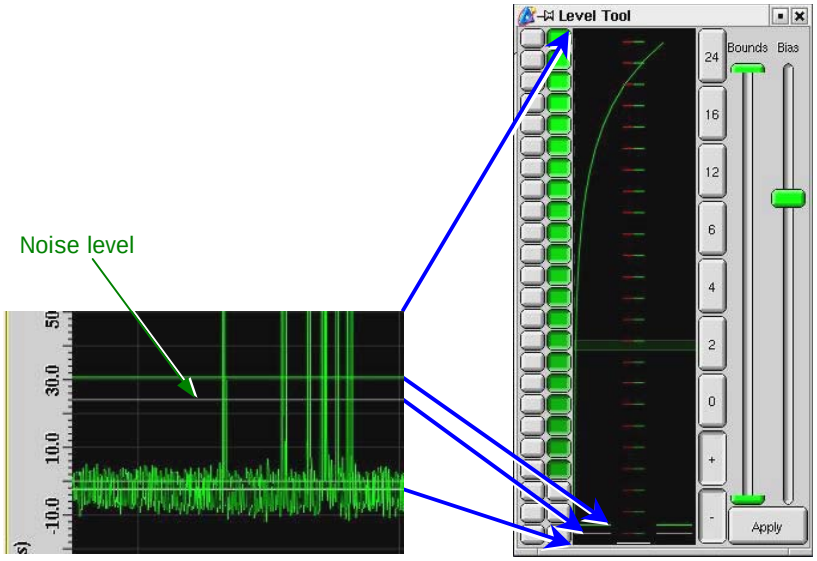
Fig. 4.9 Level Tool window

Preset button	Allows you to set the number of contour lines by selecting the 2, 4, 6, 8, 12, or 24 preset button.
Contour-line level button	The level of contour can be set manually by clicking on its button to highlight it.
Top slider	Determines the maximum intensity of the contour lines.
Bottom slider	Determines the minimum intensity of the contour lines.

Bias slider	Determines the signal intensity between the ones specified by the top slider and the bottom slider. Moving the bias slider changes the slope of the middle curve shown in Fig. 4.8. Moving it upward results in drawing more contour lines at the lower level of the signal intensities.
Noise level	Automatically set after data processing is completed.
Threshold level	Automatically set after data processing is completed, and used for peak picking in 2D processing.
Base level	Zero level of the signal intensity. Set it to the lowest level in the **Level tool** window.
Apply button	Clicking on this button redraws the contour lines at the set levels.

2. Adjust the levels of the contour lines in the **Level Tool** window.

Set the minimum intensity based on the noise level. Set the number and intensity of the contour lines to be drawn between the minimum intensity and the maximum intensity in the **Level Tool** window.



Usually, few or no contour lines are set to levels below the noise level. Setting the contour level below the noise level displays the contour lines of noise, and needs a large amount of memory in the system, slowing down the processing of the program.

Set the levels according to the following procedure:

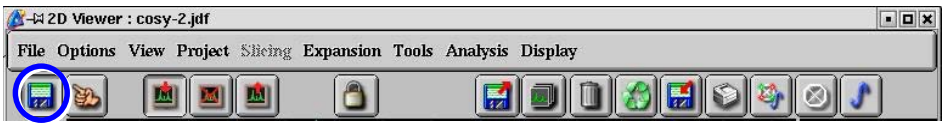
a. Click on the bottom contour-line level button.
b. Determine the bottom level of the contour lines using the bottom slider.
c. Determine the top level of the contour lines using the top slider.
d. Select the number of contour lines you want to display from the preset buttons.
e. Click on the **Apply** button.

4.3.3 Pasting 1D NMR Data

This section explains how to paste 1D NMR data onto the slice or projection data display area in the **2D Viewer** window.
It is assumed that 1D NMR data on which data processing such as FFT was already performed is stored on the hard disk or is displayed in the **1D Processor** window.

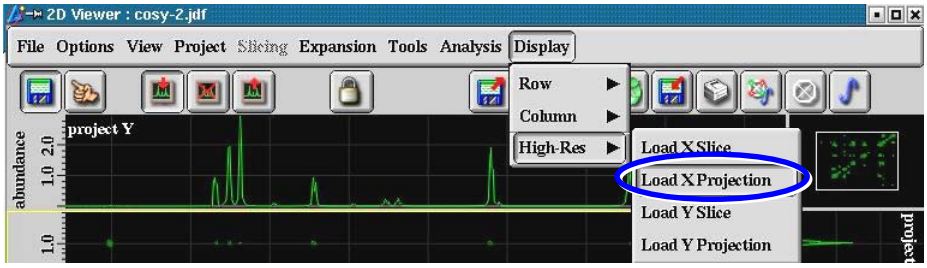
■ When 1D NMR data is stored on the hard disk

1. Click on the button.

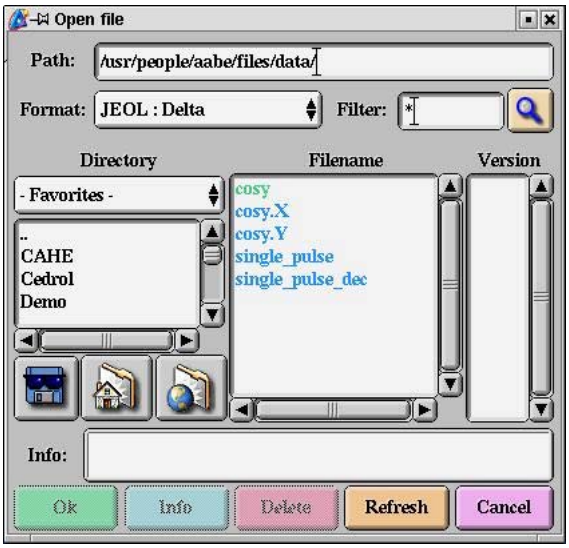


2. To paste 1D data onto the X axis:

a. Select **Display** – **High-Res** – **Load X Projection**.



The **Open Data for Processing** window opens.



b. Select a file.
ID NMR data is pasted in the projection display area of the X axis.

3. To paste 1D data onto the Y axis:

a. Select **Display** – **High-Res** – **Load Y Projection**.

b. Select a file.
1D NMR data is pasted onto the projection display area of the Y axis.

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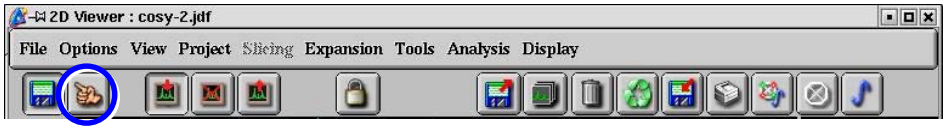
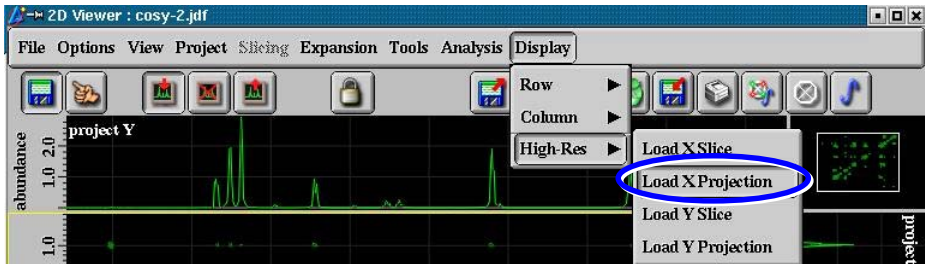
■ When 1D NMR data is displayed on the 1D Processor window

1. Click on the button.



2. To paste 1D data onto the X axis.

a. Select **Display** – **High-Res** – **Load X Projection**.



The mouse pointer changes to .

b. Move the mouse pointer onto the displayed 1D NMR data and click on it.

The 1D NMR data is pasted onto the slice or projection display area of the X-axis.

3. To paste 1D data onto the Y axis.

a. Select **Display** – **High-Res** – **Load Y Projection**.

The mouse pointer will be changed to a finger shape.

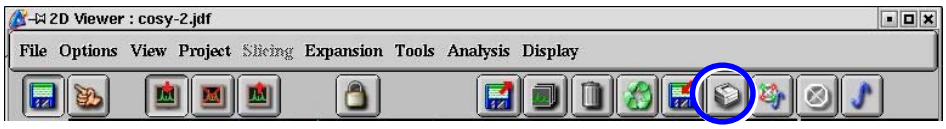
b. Move the mouse button on the displayed 1D data and click.

1D NMR data is pasted onto the projection display area of the Y axis.

4.3.4 Plotting

This section explains how to perform the standard plotting.
For the details about the settings, refer to the separate volume, Processing User's Guide.

◆ Click on the button in the **2D Viewer** window.



The default plotting is performed.

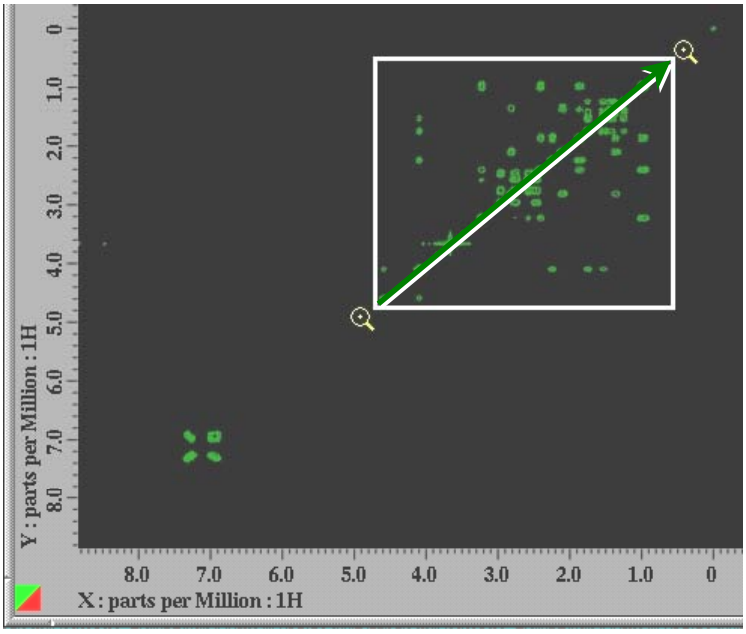
4.3.5 Changing the Display Ranges

The Cursor Tool bar is used to expand and reduce spectra.

☞ For how to display the Cursor Tool, refer to Section 3.3.4. For the details of the Cursor Tool, refer to the separate volume, Processing User's Guide.

■ To expand a spectrum vertically and horizontally at the same time

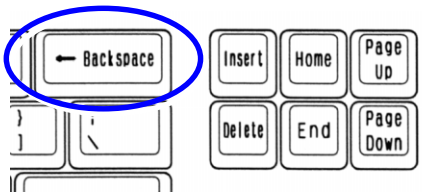
1. Select the **Zoom** mode from the Cursor Tool or press the F1 key on the keyboard.
   The Cursor Tool mode becomes **Zoom.**
2. Move the mouse pointer to the position that will become the lower left corner of expansion in the display area.
3. Press and hold down the left mouse button, and move the mouse pointer to the position that will become the upper left corner of expansion in the display area.



4. Release the left mouse button.
   The spectrum is expanded vertically and horizontally at the same time.

■ To return the spectrum display to its previous conditions

◆ Press the Backspace key on the keyboard to return the display to its previous conditions.
You can do this up to 16 times.



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When you do this, both vertical and horizontal expansions return to their previous values.
You cannot selectively return only the vertical or horizontal size to its previous value.

To return the spectrum display to its initial conditions

- Press the Home key on the keyboard.

  The horizontal and vertical scales return to their initial values.

5

QUEUING

This chapter explains how to start measurement and how to control queues.

5.1 COMMAND FOR STARTING MEASUREMENT..... 5-1
5.2 QUEUING..... 5-2

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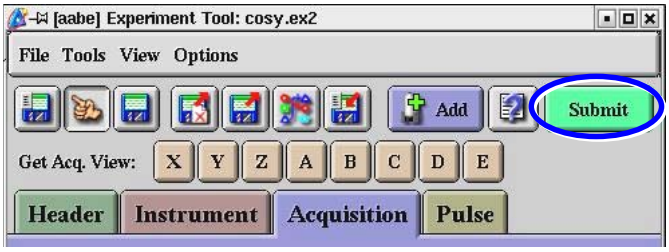
5.1 COMMAND FOR STARTING MEASUREMENT

■ Starting measurement and displaying the present status

Clicking on the **Submit** button in the **Experiment Tool** window enters the measurement into the spectrometer-control computer's queue, and the spectrometer executes measurement on a first-in, first-out basis.



The command for starting measurement can be issued repeatedly, even if another measurement is being performed. After one measurement finishes, the next measurement will be started under the stored measurement conditions.

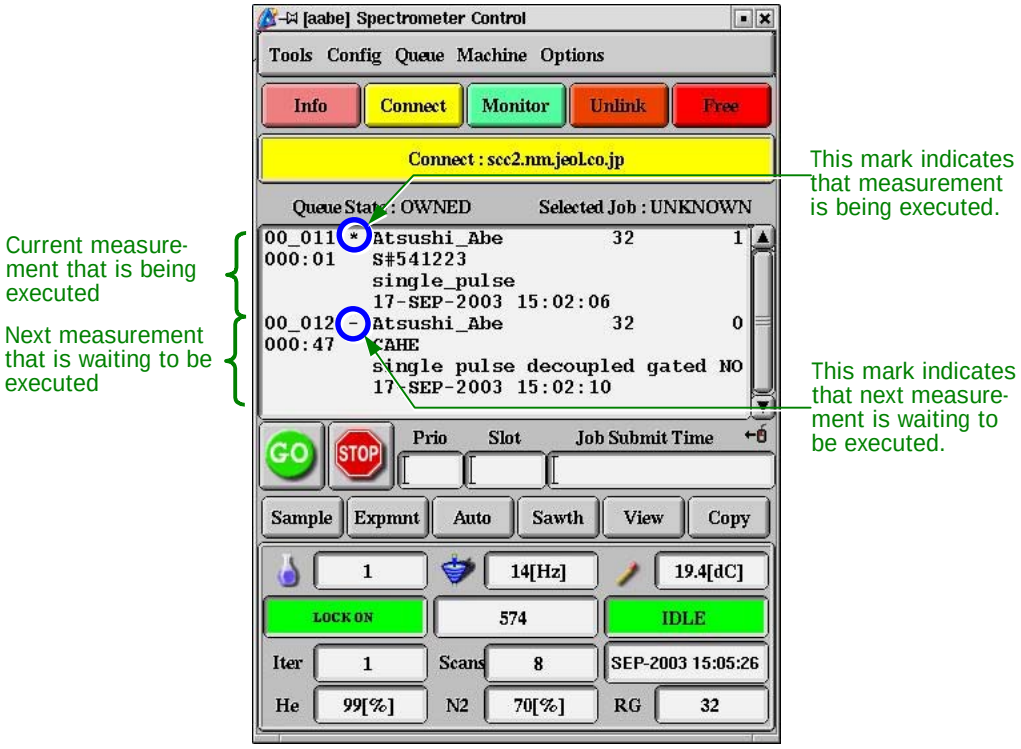


Fig. 5.1 Displaying the status of the queue

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5.2 QUEUING

■ Deleting measurement

You can delete measurements in the queue using the following procedures.

- **How to delete specified experiment**

1. Click on the measurement to delete from the **Spectrometer Control** window.
   The specified measurement is highlighted.
2. Click on the button in the **Spectrometer Control** window.
   A window appears to verify deletion.

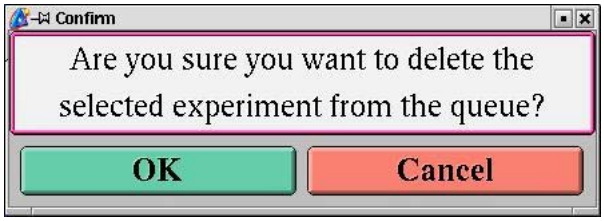
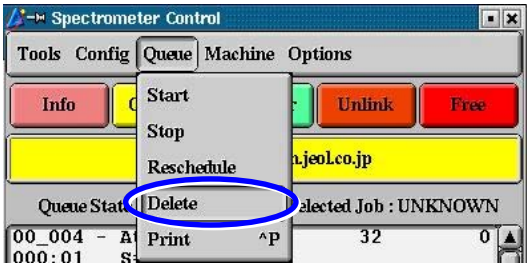


Fig. 5.2 The window that verifies the queue to delete.

3. To delete the queue, click on the **OK** button.

- **How to delete all experiment from the pending queue.**

1. Select **Queue** – **Delete** in the **Spectrometer Control** window.



A window appears to verify deletion.

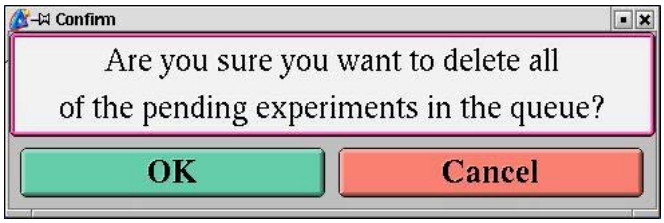


Fig. 5.3 The window that verifies the queue to delete.

2. To delete the entire queue, click on the **OK** button.

■ Viewing information about the jobs in the queue

You can view the details of a job in the measurement queue as follows.

1. Double-click on the job whose information you want to view in the **Spectrometer Control** window.
   The **Job Info** window opens.

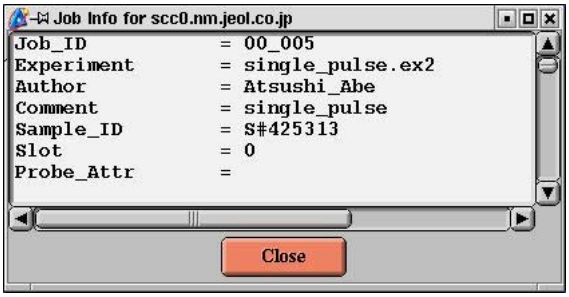


Fig. 5.4 Job Info window

2. Display the parameter you want to make sure of, using the arrow ▲▼ buttons.
3. To finish viewing, click on the **Close** button.
   The **Job Info** window is closed.

SAVING AND LOADING DATA

Chapter 6 explains how to save NMR data, and how to load data from a file.

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6.1 SAVING NMR DATA

6.1.1 Saving the measured data (FID)

The measured data (FID) is saved automatically. A file name for the saved data is specified as in the following procedure.

■ Specifying a file name for saved data before measurement

1. Specify the file name to the data you want to save in the **filename** of the **Experiment Tool** window.

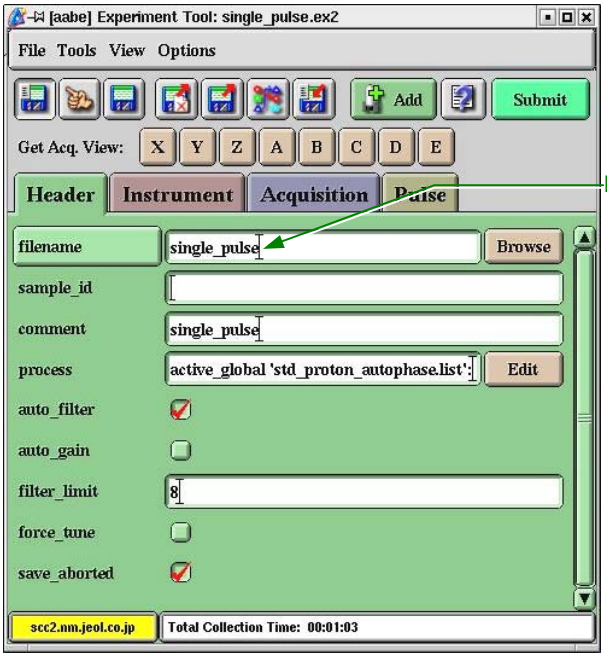

Fig. 6.1 Experiment Tool window

2. When specifying the directory to save, click on **filename** or on the **Browse** button.

The **Save Collect Data to …** window opens.

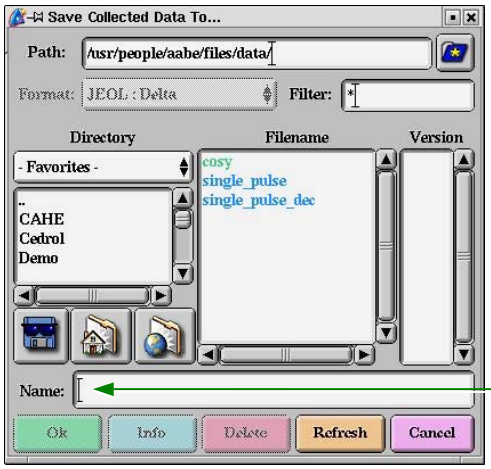

Fig. 6.2 Save Collect Data to… window

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3. After moving to the directory to save, enter the file name to save it in the **Name** entry box, and click on the **OK** button.

When creating a new directory, after specifying a directory name in the **Path** input box, click on the button. Create the directory and move it. After that, enter the filename to save it into the filename entry box.

4. Start measurement.

When measurement is complete, the data is saved with the specified name.

Specifying a saving file name after measurement

When you did not specify a filename before measurement, the measured data is saved with a **filename** specified in the **Experiment Tool** window. Change this saved filename using the following procedure.

1. Select **File–Change Working File** from the **1D Processor** or **nD Processor** window.

The **Rename Data File to...** window opens.

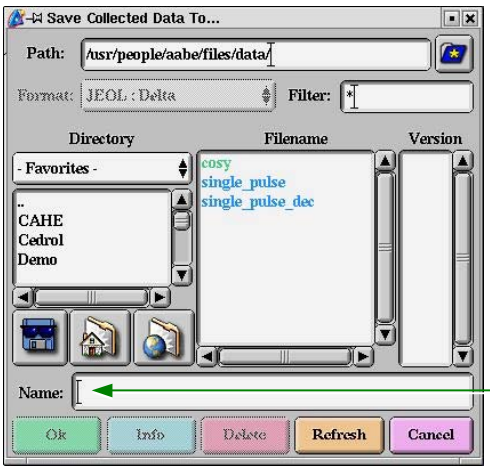

Fig. 6.3 Rename Data File to... window

2. Type any filename in the filename entry box.

When creating a new directory, after specifying a directory name in the **Path** input box, click on the button. Create the directory and move it. After that, enter the filename to save it into the filename entry box.

3. Click on the **Ok** button.

The filename of the measurement data (FID) changes to the specified filename.
If that filename exists, the version number is incremented by one.

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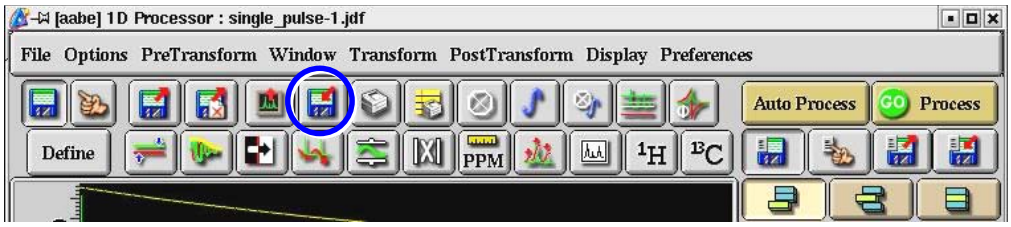
6.1.2 Saving Processed Data

■ To save 1D processed data in the 1D Processor window under the same filename

◆ Click on the button in the **1D Processor** window.



The 1D processed data is saved. Then, the version number increases automatically under the same filename.

■ To save 1D processed data in the1D Processor window under a new filename

1. Select **File** – **Save As** from the menu bar.

The **Save Data File** window opens.

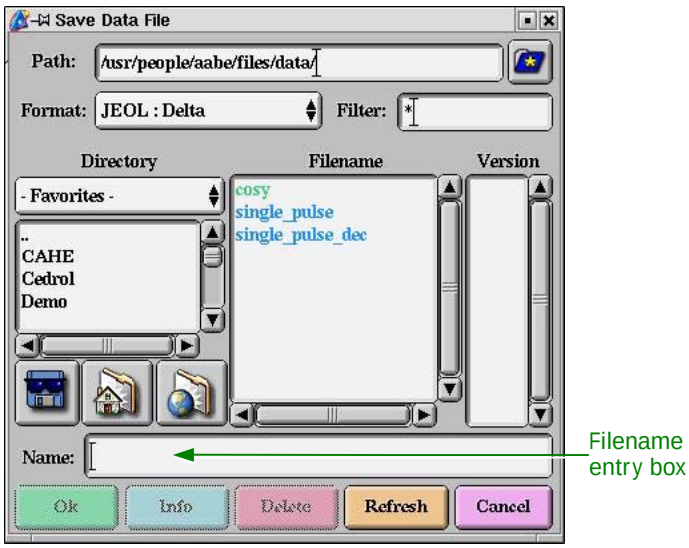


Fig. 6.4 Save Data File window

2. Type any filename in the filename entry box.

When creating a new directory, after specifying a directory name in the **Path** input box, click on the button. Create the directory and move it. After that, enter the filename to save it into the filename entry box.

3. Click on the **Ok** button.

The 1D processed data is saved under the specified filename.

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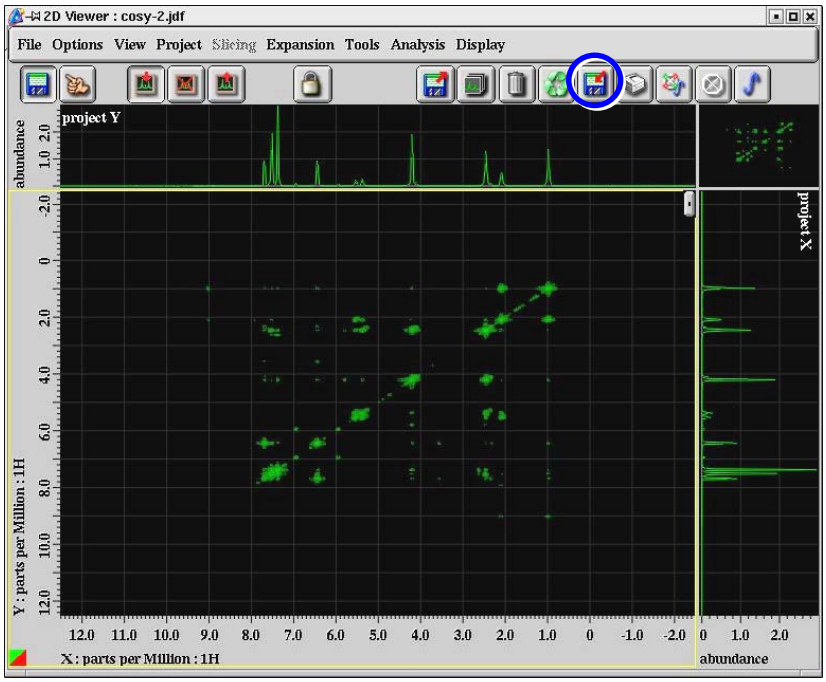
To save 2D processed data in the 2D Viewer window under the same filename

- Click on the button.


2D Viewer : cosy-2.jdf
File Options View Project Slicing Expansion Tools Analysis Display
project Y
abundance
project X
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

The 2D processed data is saved. Then, the version number increases automatically under the same filename.

To save 2D processed data in the 2D Viewer window under a new filename

1. Select **File** – **Save As** from the menu bar.
   The **Save Data File** window opens.

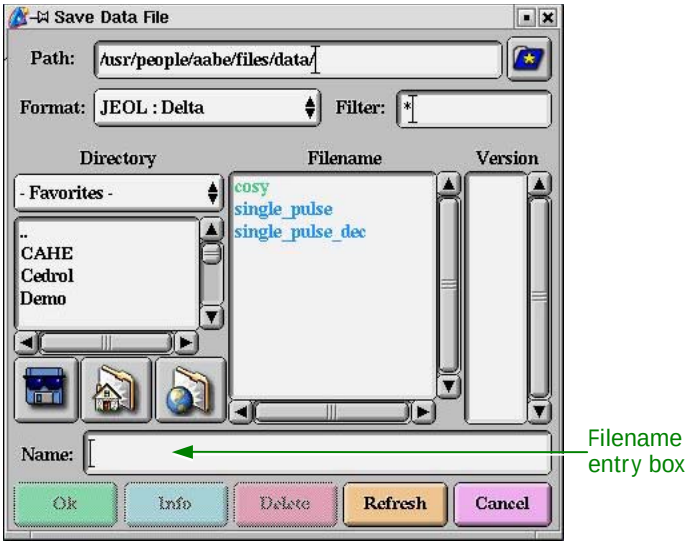


Fig. 6.5 Save Data File window

C I

2. Type any filename in the filename entry box.

When creating a new directory, after specifying a directory name in the **Path** input box, click on the button. Create the directory and move it. After that, enter the filename to save it into the filename entry box.

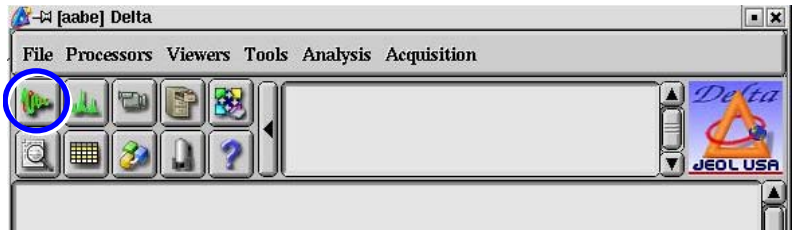
3. Click on the **Ok** button.

The 2D processed data is saved under the specified filename.

C I

6.2 LOADING DATA

1. Click on the button in the **Delta Console** window.



The **Open Data for Processing** window opens.

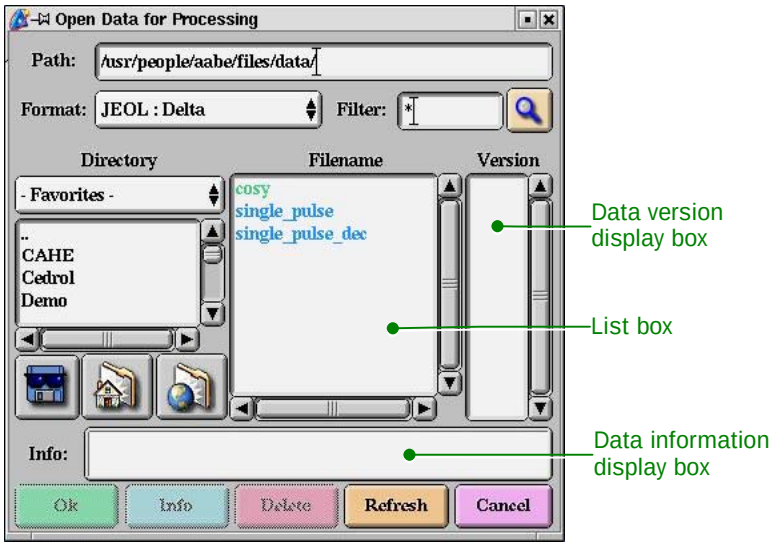


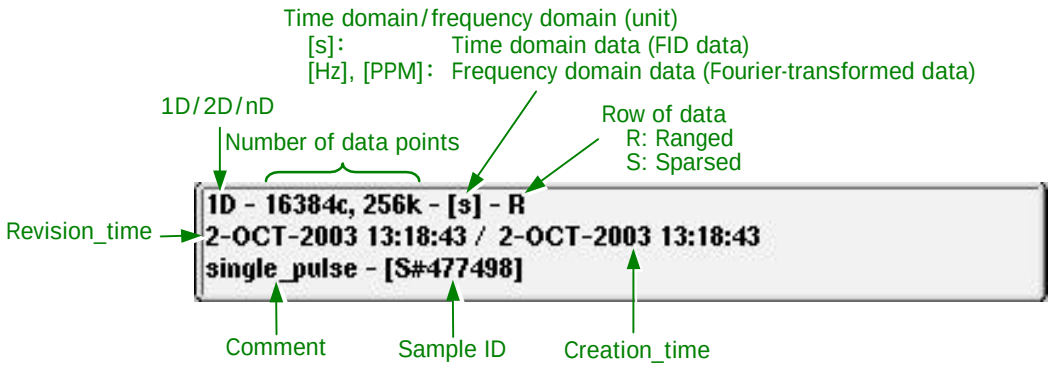
Fig. 6.6 Open Data for Processing window

2. Click on the name of the data file you want to load in the list box.

3. Click on the **Ok** button.

The most recent version of data is displayed in the **1D Processor** window or **nD Processor** window.

The following information on the most recent version of data is displayed in the data information display box.



If you want to display earlier data, select the version number, referring to information in the data information display box, and click on the **Ok** button.

Version number

In the Delta program, a version number is appended to each data filename. Before data is processed, a new file is automatically created under the same filename with a different version than that of the original data. The original data is not processed, preventing corruption of the original FID data. If you save data under the existing filename, the data is given a version number one higher. Copied data is sometimes deleted after it is processed. Therefore, some of the version numbers in the file list are usually omitted.

Directory

You can specify two directories in the **Open Data for 1D Processor** window using the buttons. One is a local directory. The other is a global directory. Normally, the user uses the local directory.

Local directory

Clicking on the button displays a list of the files in the local directory in the middle of the **Open Data for 1D Processor** window.

✍ The local directory is specified in **DATA** in the **.delta_configure** file.

Global directory

Clicking on the button displays a list of the files in the global directory in the middle of the **Open Data for 1D Processor** window. Because the global directory cannot be used for writing, it is not used to store data.

✍ The global directory is specified in **GLOBAL** in the **.delta_configure** file.

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